LaMCoS
Laboratoire de Mécanique
des Contacts et des Structures
UMR 5259

Habilitation à Diriger des Recherches

The role of length scales in material failure

Gergely Molnár

Jury

Rapporteurs:	*Samuel Forest - Mines Paris PSL CNRS*
	David Rodney – UBCL1
	Jean-François Molinari - EPFL
Examinatrice:	*Laura De Lorenzis - ETH Zürich*
Examinateurs:	*Nicolas Moës - UCLouvain*
	Anthony Gravouil - INSA Lyon

Lyon, France

05/03/2025

Phase-field

symmetric

Video and experiment by Rian Seghir (GeM)

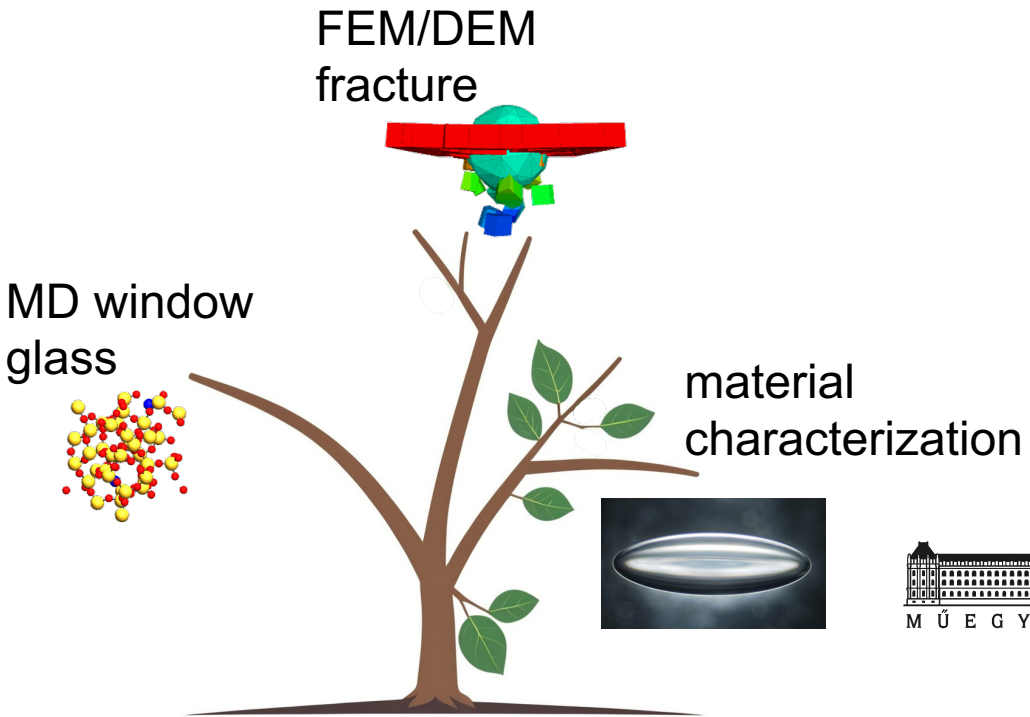
Introduction

My journey

Ph.D.

2011-2014

Multi-scale modelling of structural glass



Introduction

Postdocs

2014-2018

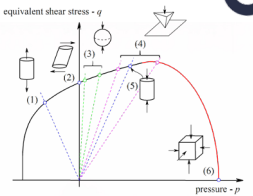
My journey

cellulose MD + DEM

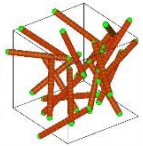
UGA

INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON

atomistic yield criterion



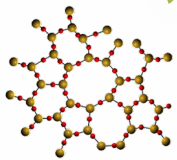
MINES Saint-Étienne



phase-field fracture

dynamic fracture

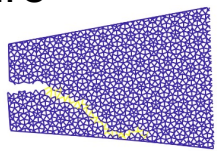
micro-scale analysis



UNIVERSITÉ DE LYON

Lyon 1

Cosserat fracture



CENTRALE NANTES

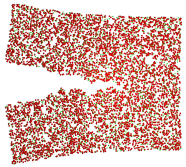
Introduction

CR CNRS

(associate professor)

2018-present

My journey



anr GaLAaD

anr RATES

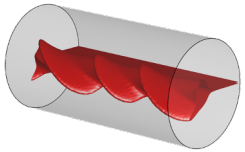
anr metamaterials

UDS

cea

IRSN

CC+PF



MatéIS Matériaux Ingénierie et Science UMR 5510

anr e-WARNINGS

Neg

anr DENSE

atomic scale simulations

fracture

- PhD / Postdoc

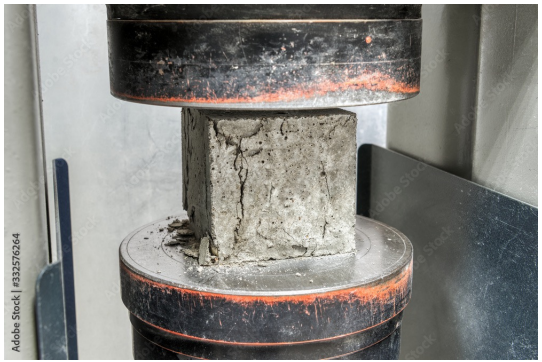
anr French National Research Agency

cnrs

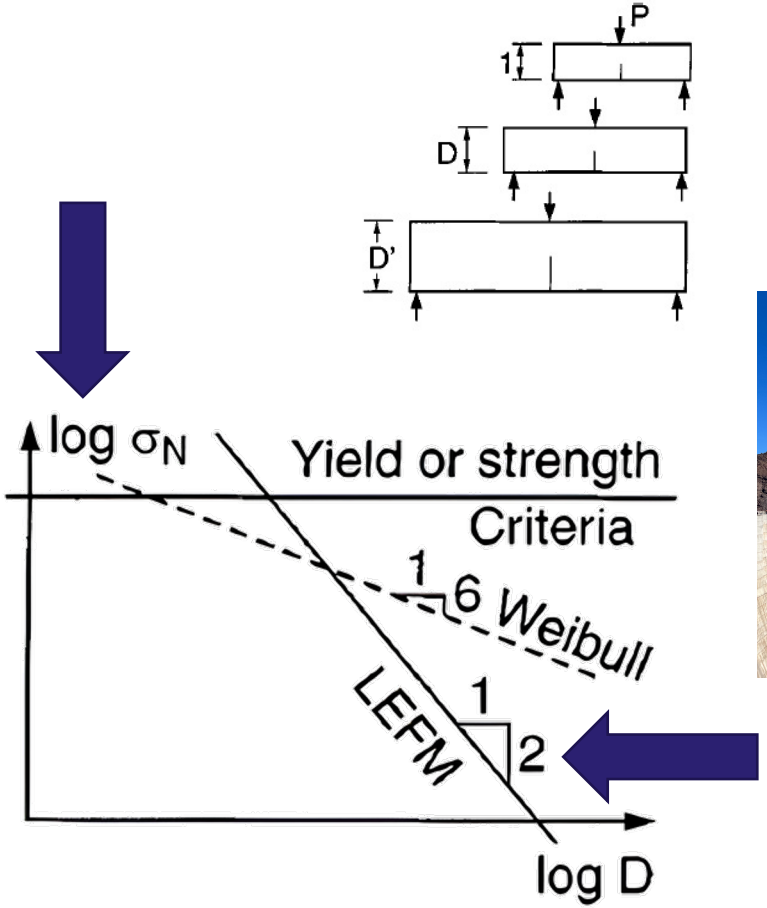
INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON

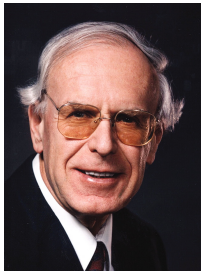
Motivation

Length scale in failure



Laboratory testing





Bažant et al. (1999)

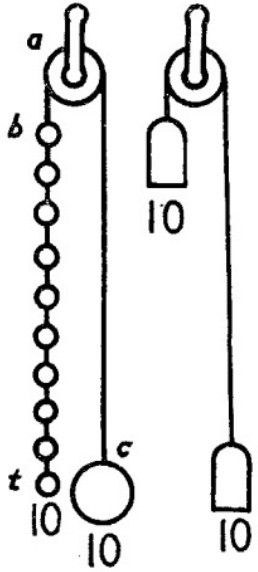
Hoover dam

Motivation

History

1500's

(Codex Atlanticus, Leonardo da Vinci)

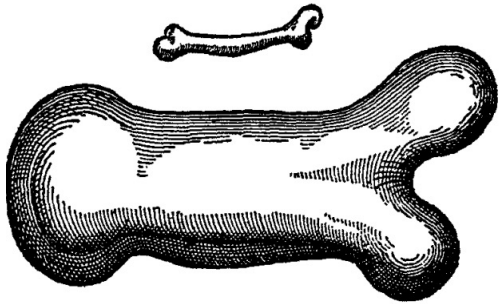


"among cords of equal thickness the **longest** is the **least strong**…"

"a cord is so much **stronger**…as it is **shorter**"

1638

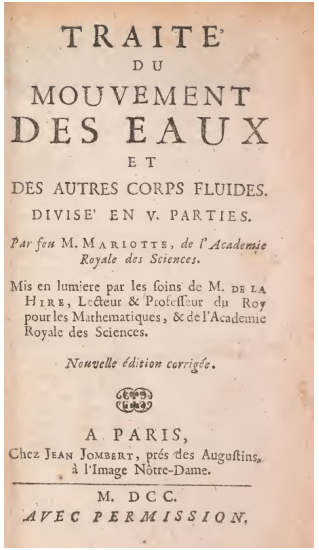
(Two New Sciences, Galileo Galilei)



"…the **smaller** the body the **greater** its relative **strength**"

(Traité du mouvement des eaux, Edmé Mariotte)

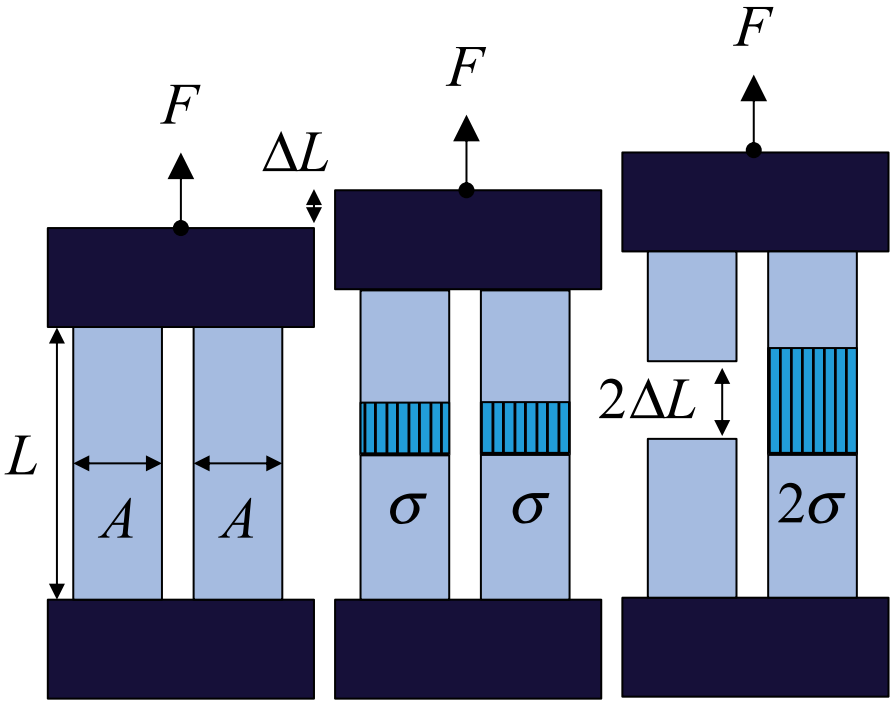
1686


TRAITE'
DU
MOUVEMENT
DES EAUX
ET
DES AUTRES CORPS FLUIDES.
DIVISE' EN V. PARTIES.
Par feu M. MARIOTTE, *de l'Academie Royale des Sciences.*
Mis en lumiere par les soins de M. DE LA HIRE, Lecteur & Professeur du Roy pour les Mathematiques, & de l'Academie Royale des Sciences.
Nouvelle édition corrigée.
A PARIS,
Chez JEAN JOMBERT, prés des Augustins, à l'Image Nôtre-Dame.
M. DCC.
AVEC PERMISSION.

"A long rope and a short one always support the same weight, unless that in a long rope there may happen to be some **faulty place**, in which it will break sooner than in a shorter."

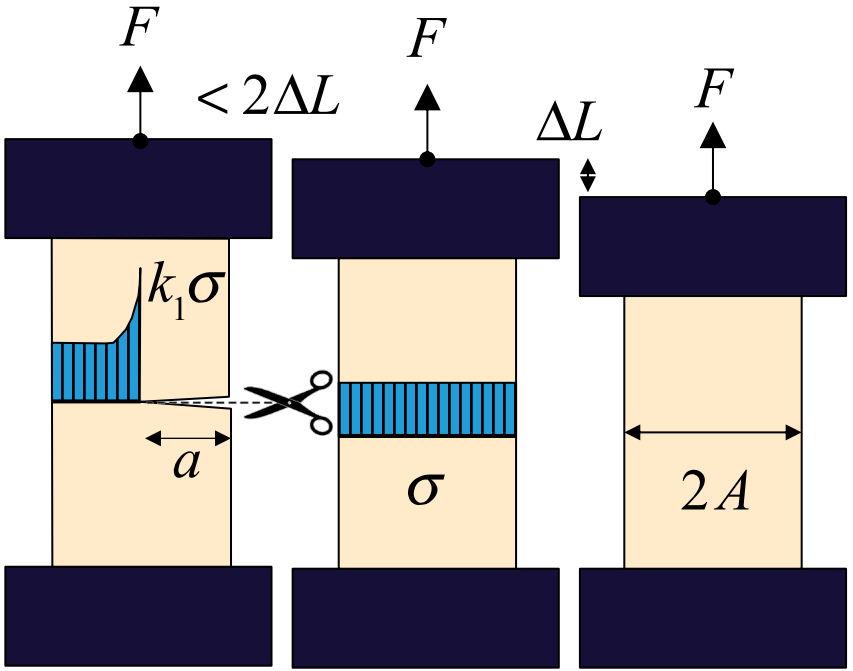
Motivation

Classical mechanics



$$\sigma = \frac{F}{2A}$$

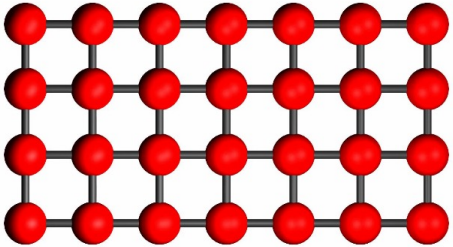
Fracture mechanics

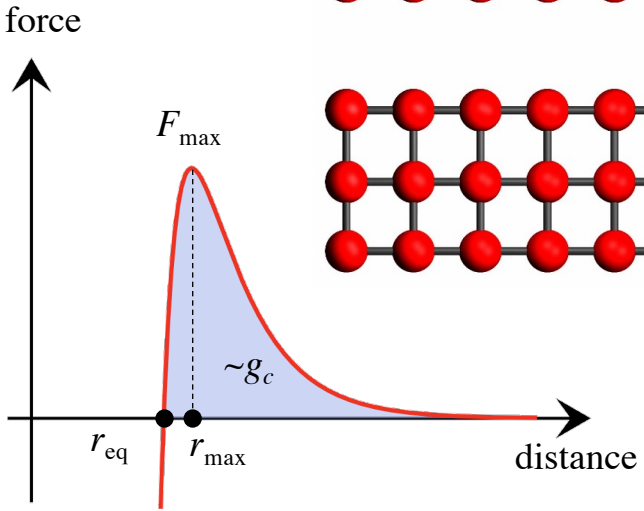


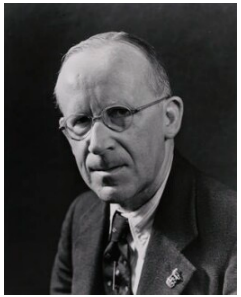
$$\sigma = \frac{F\sqrt{\pi a}}{2A}\frac{1}{\sqrt{2\pi r}}g(\theta)$$

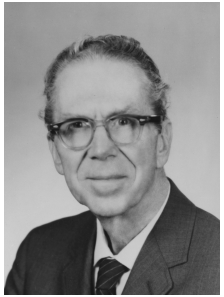
Motivation

Energy release rate / Toughness





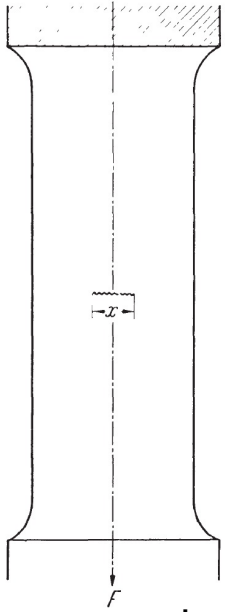


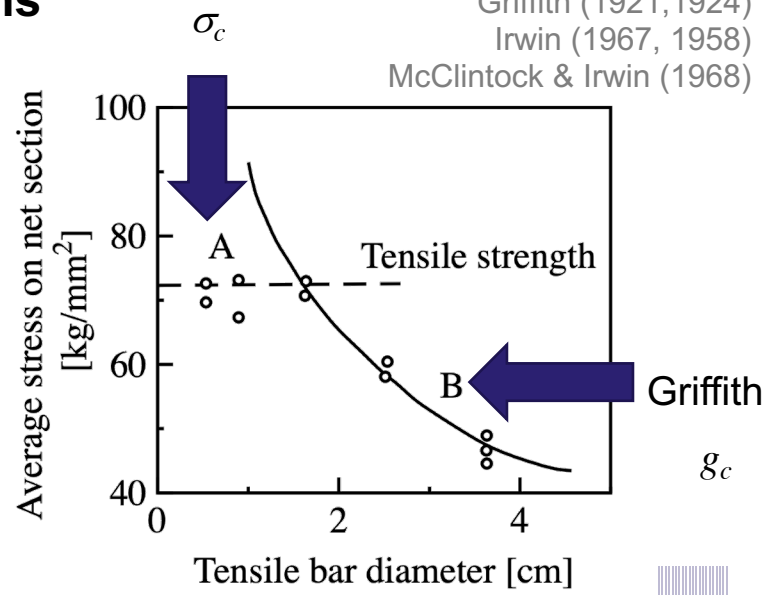


Griffith (1921,1924)
Irwin (1967, 1958)
McClintock & Irwin (1968)

strength

Limitations

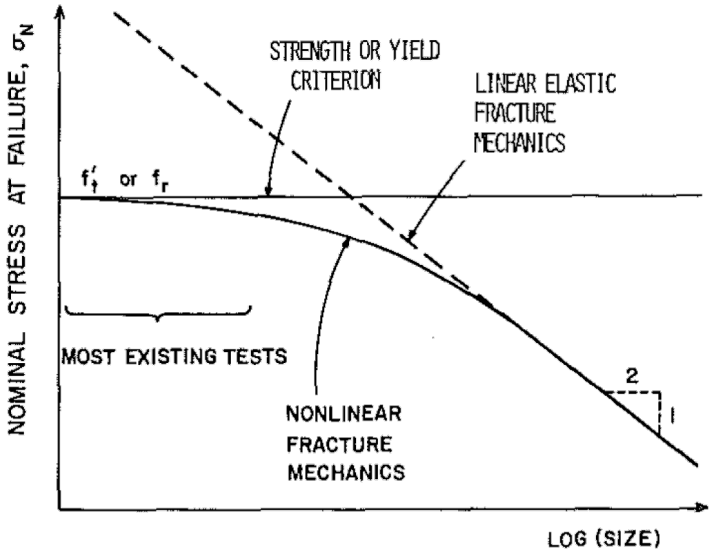




Irwin's length $l_{mat} = \frac{Eg_c}{\sigma_c^2}$

Motivation

Length scale in failure

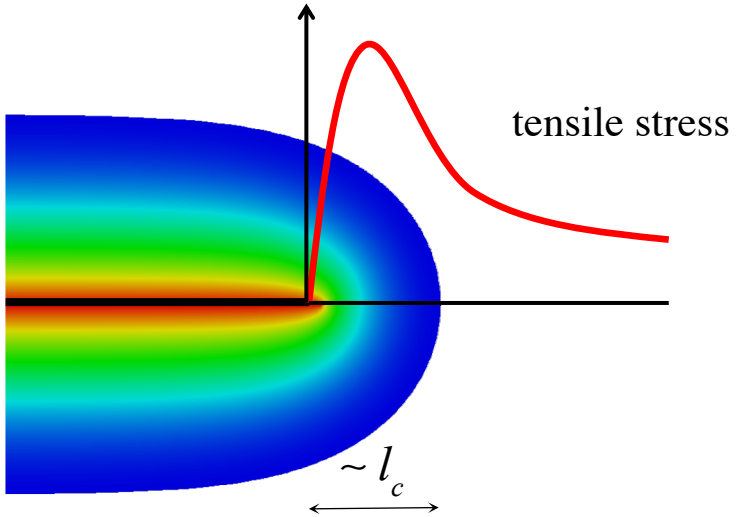


(Bažant et al., 1984)

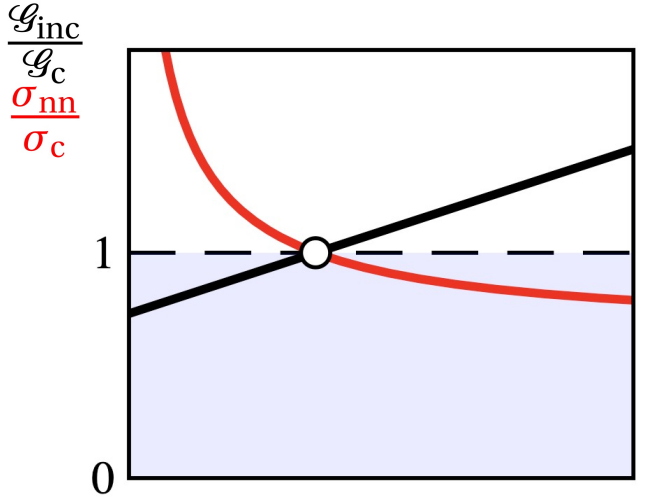
- concrete — Shah & Swartz (1987)
- composites — Bažant et al. (1996)
- rocks — Bažant et al. (2004)
- ceramics — Usami et al. (1986)
- silica glass — Luo et al. (2016)
- wood — Simon (2009)
- SiC — Bažant et al. (1990)
- sea ice — Dempsey et al. (1995)
- alumina — Leguillon et al. (2018)
- etc…

Continuum Fracture

Phase-field model

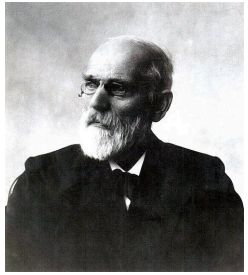


Coupled criterion



Continuum Fracture

Phase-field approach



liquid–gas interfaces with **density functions**

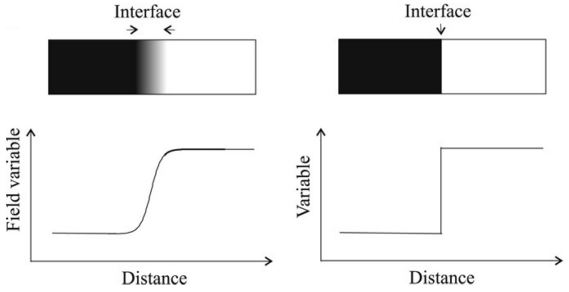
van der Waals (~1900)

superconductivity

(Ginzburg & Landau, 1950)

diffuse interfaces

(Cahn & Hilliard, 1958)



L. M. Kachanov (1958)

continuum damage mechanics

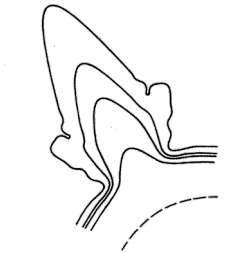
$$\psi = \frac{1}{2}(1-d)\varepsilon_{ij} C_{ijkl} \varepsilon_{kl}$$

- fracture mechanics

(Bourdin et al., 2000)

- solidification

- image processing (Fix, 1983) (Langer, 1986)



Continuum Fracture

Phase-field approach

1. Brittle fracture $$-\frac{\partial \psi}{\partial a} = \frac{\partial S}{\partial a} = g_c$$ (Griffith, 1920)

(Bourdin et al., 2000)

2. Minimization problem $$\Pi(\mathbf{u},\Gamma) = \int_\Omega \psi\left(\varepsilon(\mathbf{u})\right) d\Omega + g_c \int_\Gamma d\Gamma$$

(Mumford & Shah, 1989)
(Francfort & Marigo, 1998)

3. Crack energy density

crack energy density

$$\Pi(\mathbf{u},d) = \int_\Omega g(d)\psi_0\left(\varepsilon(\mathbf{u})\right) d\Omega + \int_\Omega \frac{g_c}{c_\omega l_c}\left(\omega(d) + l_c^2 |\nabla d|^2\right) d\Omega$$

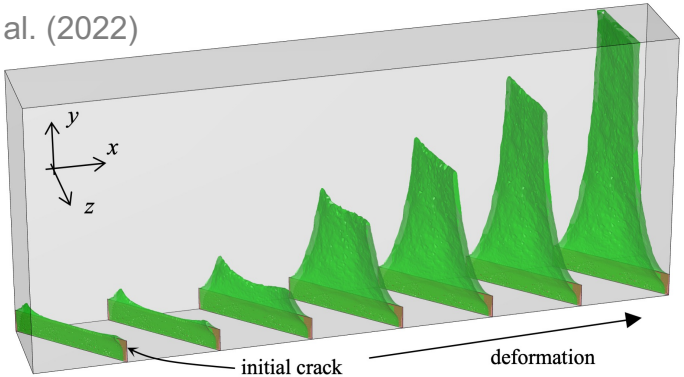
$$l_c \to 0 \quad \Gamma \text{ converges}$$

(Ambrosio & Tortorelli, 1990)
(Bourdin et al., 2000)
(Amor et al., 2009)
(Miehe et al., 2010)

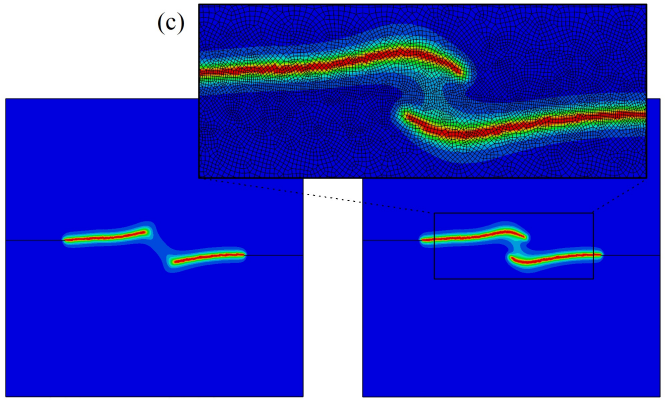
Continuum Fracture

Phase-field approach - Examples

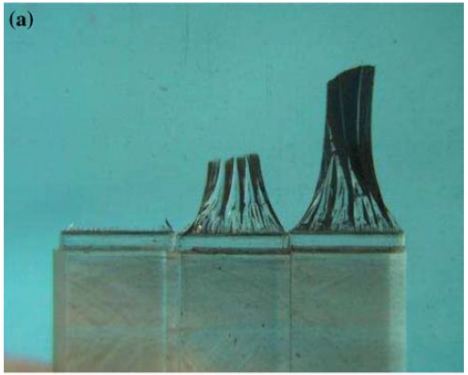
Molnár et al. (2022)



Molnár et al. (2017)



Solving **fracture mechanics** problems with Partial Differential Equations (**PDE**s)



Mode I+III

Lazarus et al. (2008)

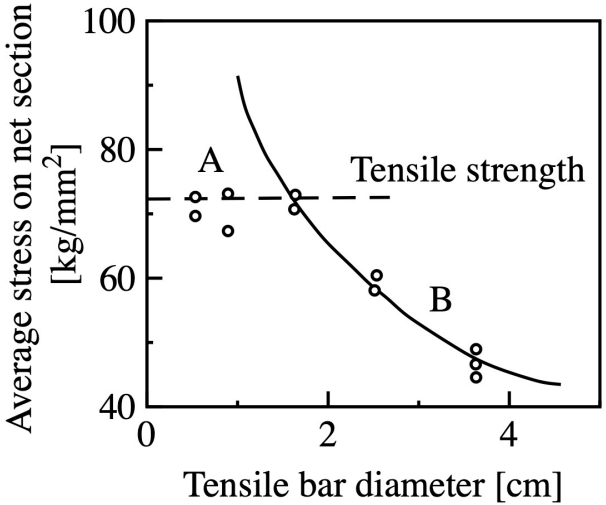
Mode I+II

Continuum Fracture

Length scale in fracture

Tensile opening

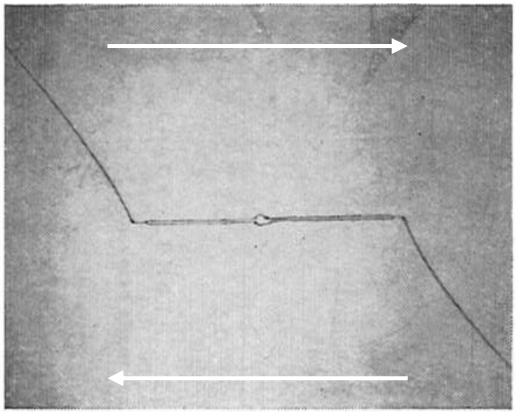
Mode I



(Irwin, 1958)
(Lubahn, 1956)

In-plane shear

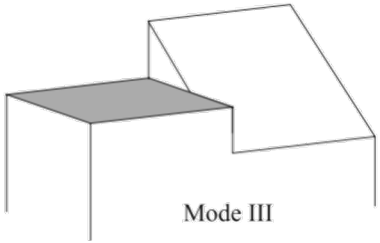
Mode II

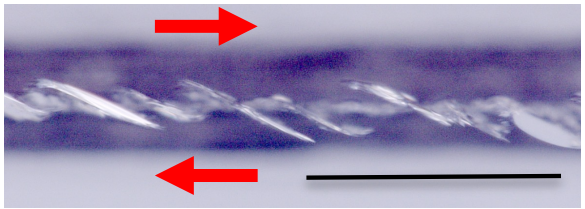


(Erdogan & Sih, 1963)

Antiplane shear

Mode III

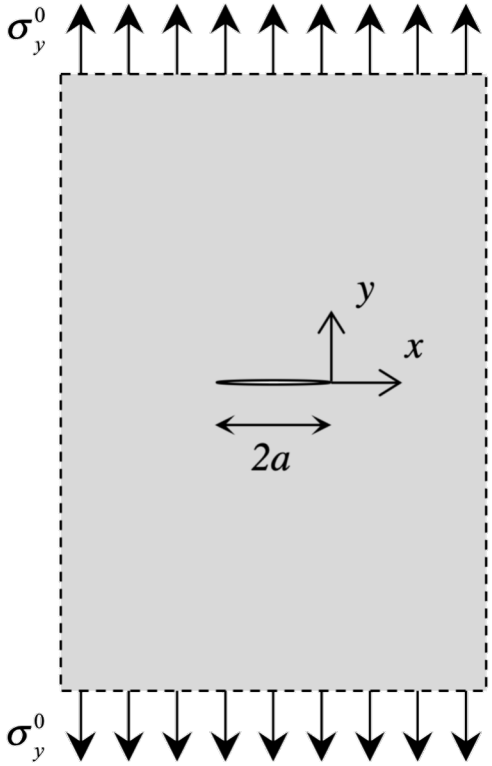


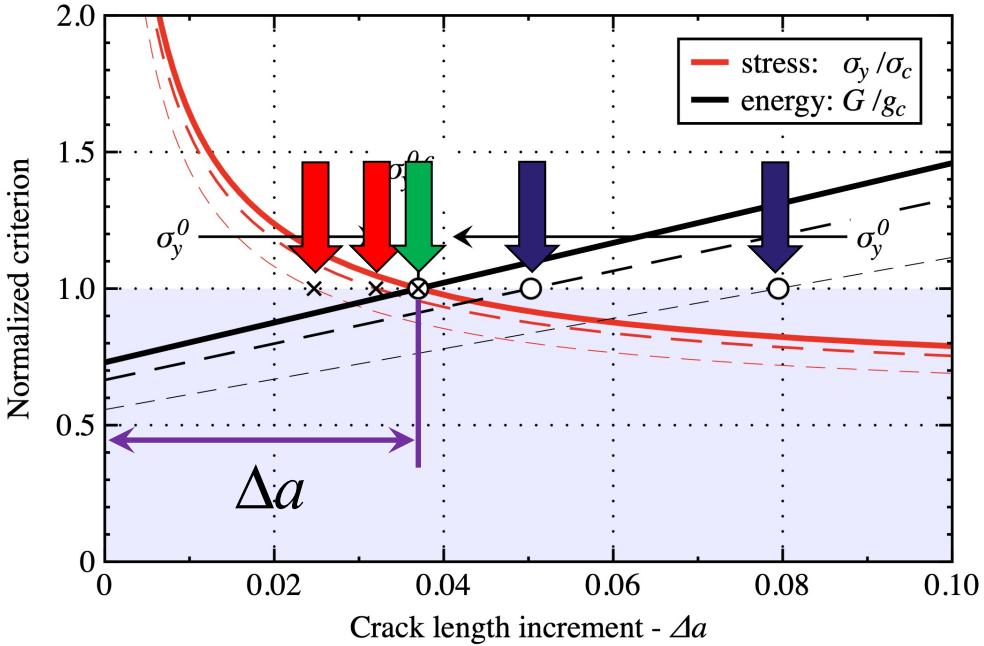


(Sommer, 1969)
(Chen et al., 2015)

Continuum Fracture

Finite fracture mechanics





Leguillon (2002)

$$\frac{\partial \Pi}{\partial a} \geq g_c$$

Griffith

Stress

$$\sigma_1\left(a+\Delta a\right) \geq \sigma_c$$

Molnár et al. (2020)

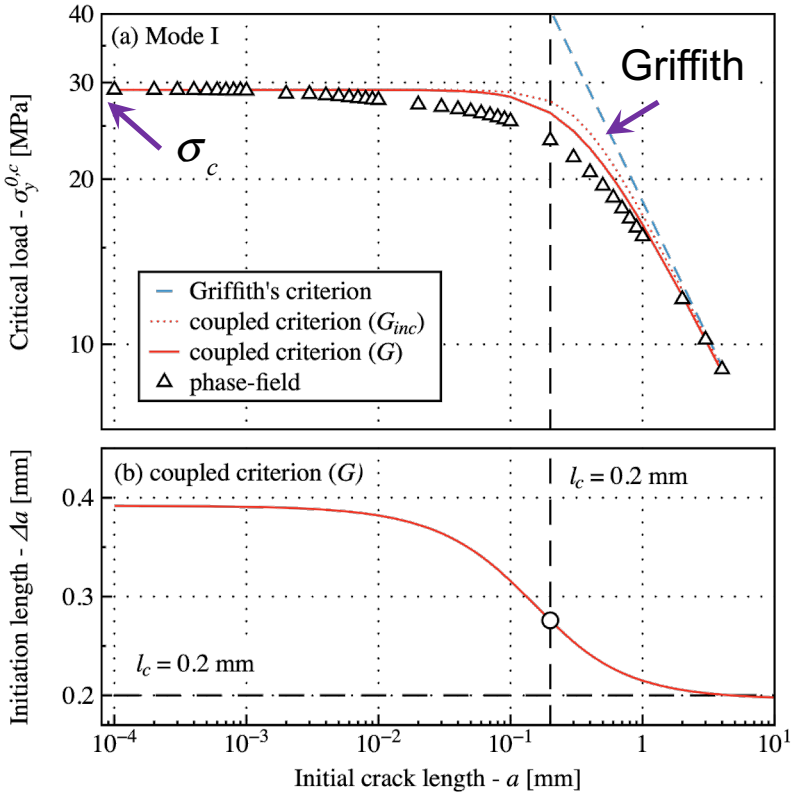
Coupled *stress* and *energy* criteria

Continuum Fracture

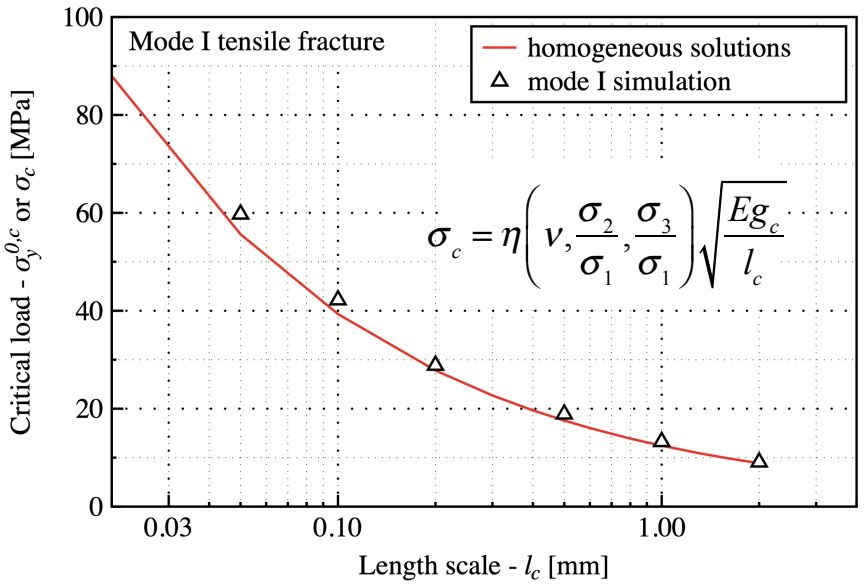
Molnár et al. (2020)

Tensile opening

Size effect



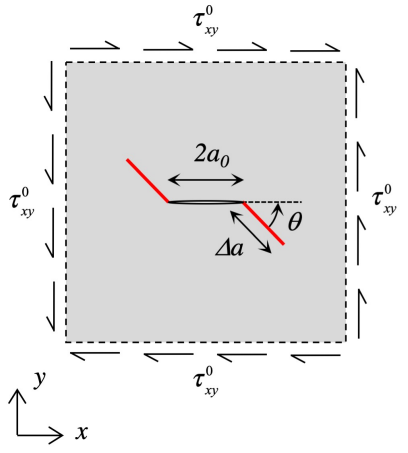
Correlation



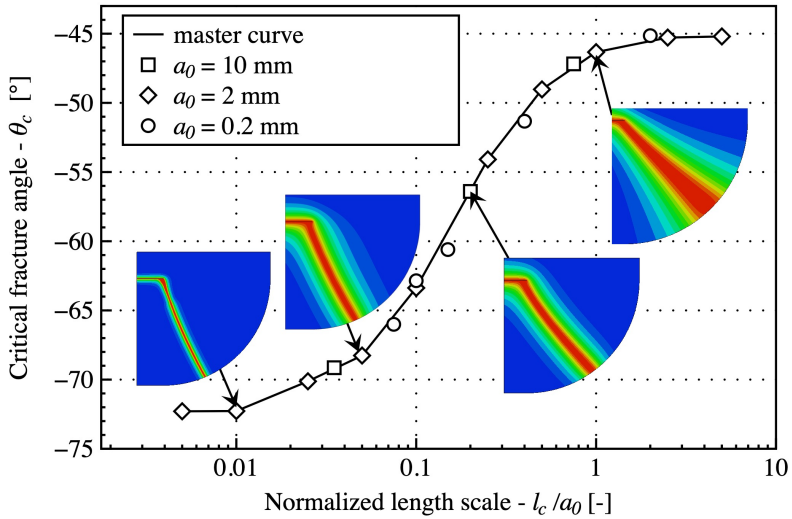
Continuum Fracture

In-plane shear fracture

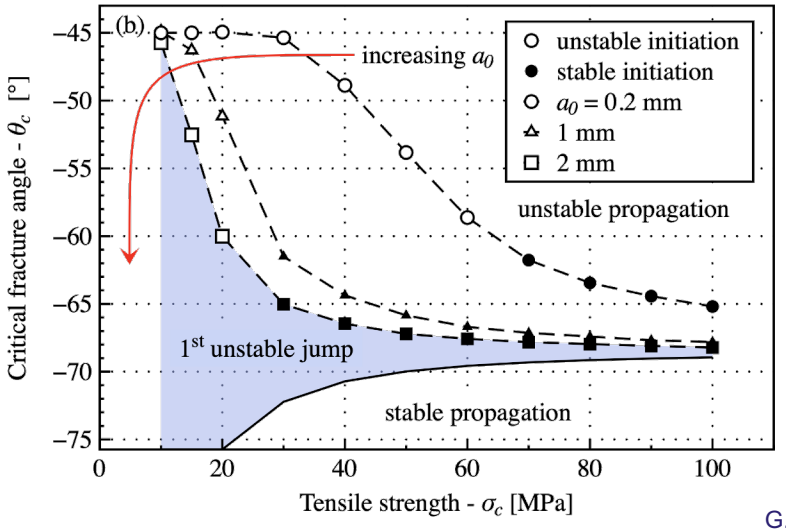
Molnár et al. (2020)



Phase-field



Coupled criterion



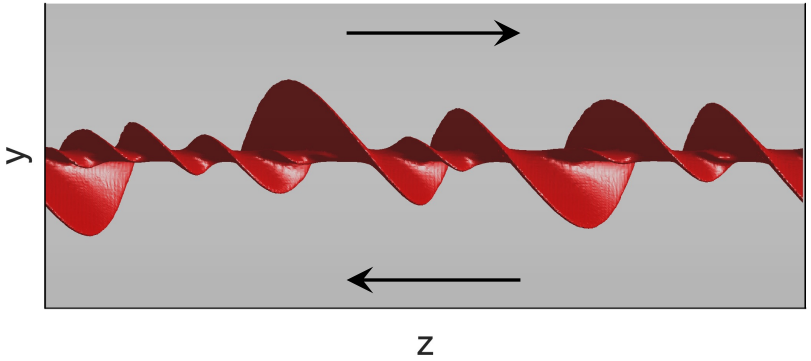
Continuum Fracture

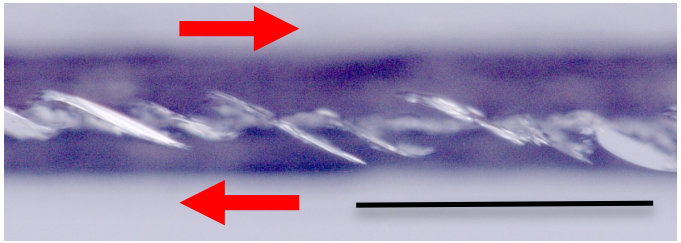
Antiplane echelon cracking

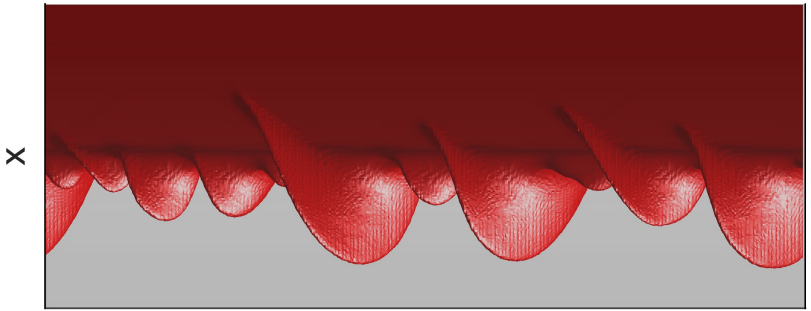
Madeira, Portugal (2022)

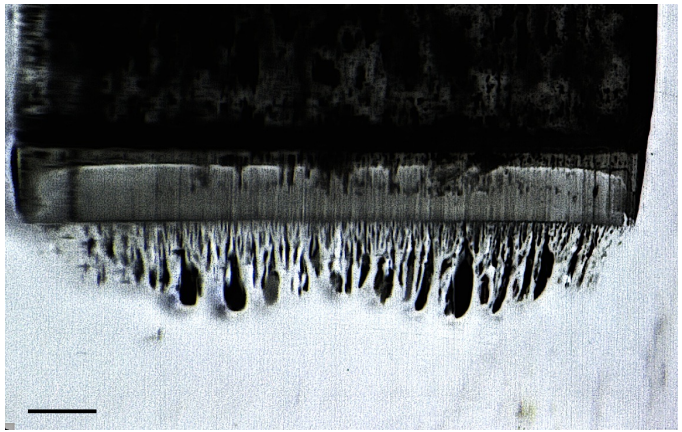
Continuum Fracture

Antiplane echelon cracking









Molnár et al. (2024)

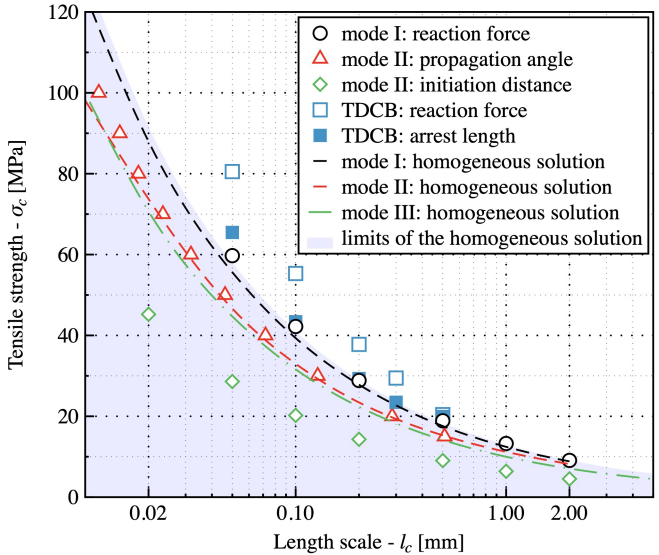
(Chen et al., 2015)

Continuum Fracture

Molnár et al. (2020)
Molnár et al. (2024)

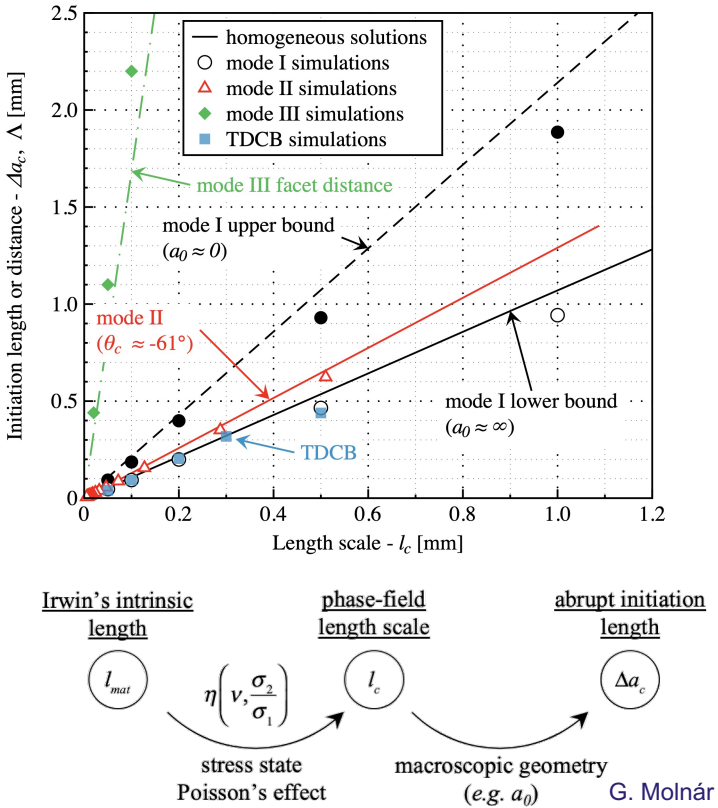
Length vs strength

Strength



$$\sigma^{\max} = \eta\left(\nu, \frac{\sigma_2}{\sigma_1}, \frac{\sigma_3}{\sigma_1}\right)\sqrt{\frac{Eg_c}{l_c}}$$

Initiation length



Continuum Fracture

(PMMA, v = 25 m/s)

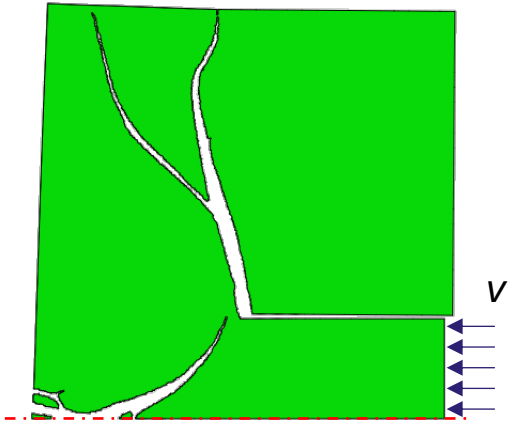
Dynamic fracture

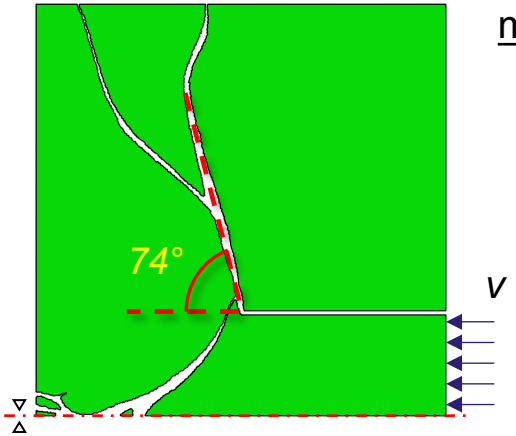
(Molnár et al., 2022)

Kinetic energy

$$\mathcal{L} = D\left(\dot{\mathbf{u}}\right) - \Pi\left(\mathbf{u}, d\right)$$

$$D\left(\dot{\mathbf{u}}\right) = \frac{1}{2}\int_{\Omega} \dot{\mathbf{u}}^T \dot{\mathbf{u}} \rho \, d\Omega$$

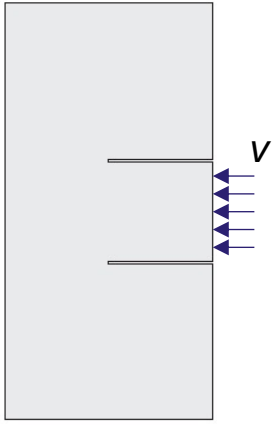


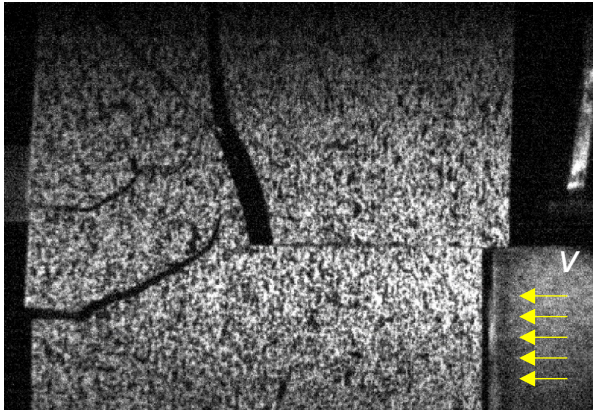


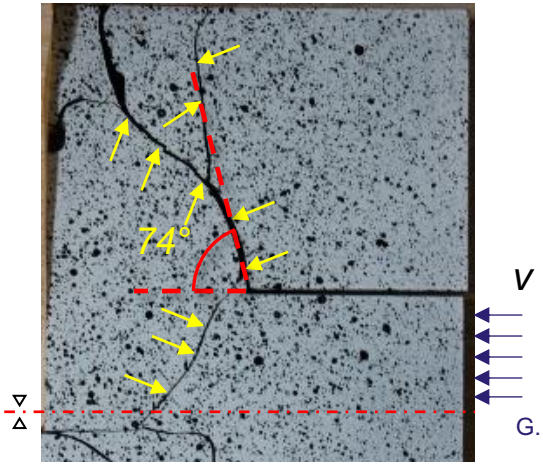
material

E = 6 GPa

g_c = 600 J/m^2



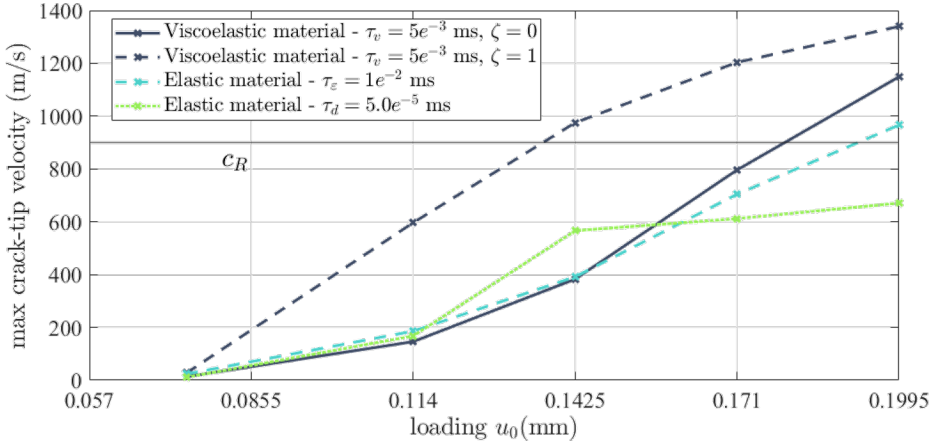




Continuum Fracture

Dynamic fracture - viscoelasticity

Crack tip velocity

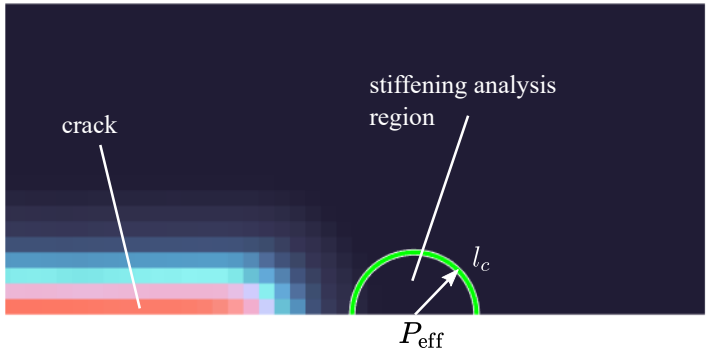


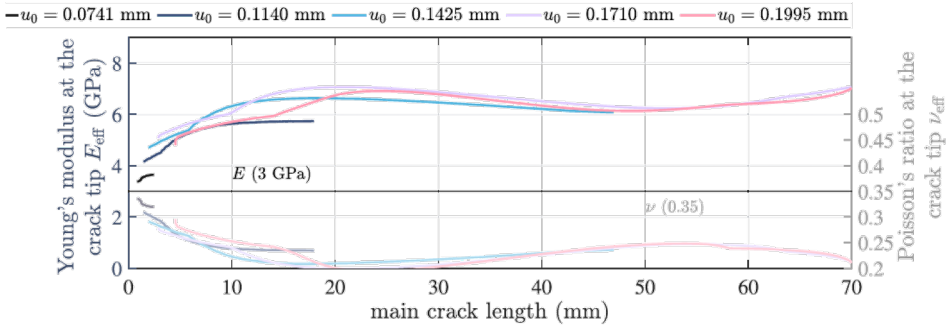
$$\Pi(\mathbf{u},d) = \Pi_{el}(\mathbf{u},d) + \Pi_d(d) +$$

$$+ \int_{\Omega}\int_{-\infty}^{t} \boldsymbol{\sigma}_v(\dot{\boldsymbol{\varepsilon}}_v, d) : \dot{\boldsymbol{\varepsilon}}_v \, d\tau \, d\Omega$$

Eid et al. (2023)

Local stiffness

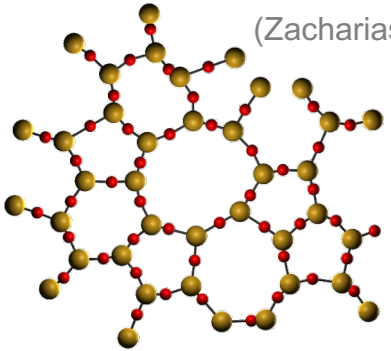




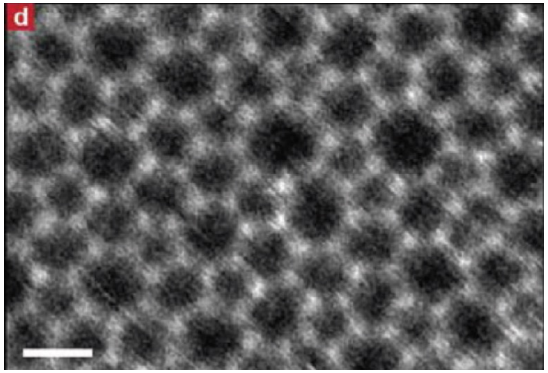
Resistance of Silicate Glasses

Molnár et al. (2016)

Silicate glasses

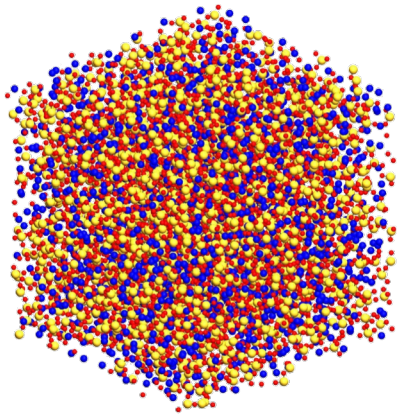


(Zachariasen, 1932)



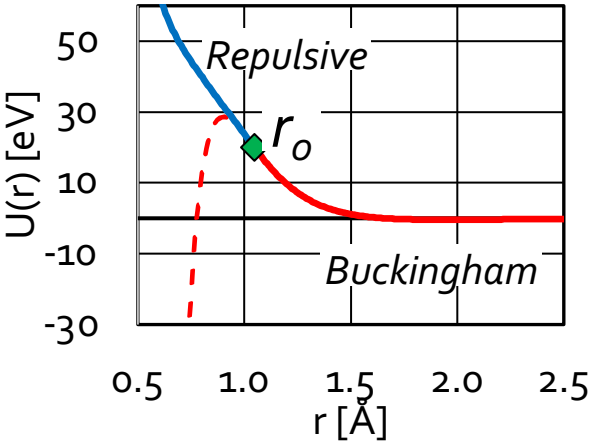
Atomic-resolution electron spectroscopy (Huang et al., 2012)

Atomic scale simulations



1. BKS Interaction potential
2. Initial sample generation (random → heat → quench → SiO_2-xNa_2O)
3. Verification (diffraction, NMR, Brillouin)
4. Athermal deformation

Potential function



$$U_{BKS}\left(r_{ij}\right) = k\frac{q_i q_j}{r_{ij}} + e^{-r_{ij}/\rho} - \frac{C}{r^6}$$

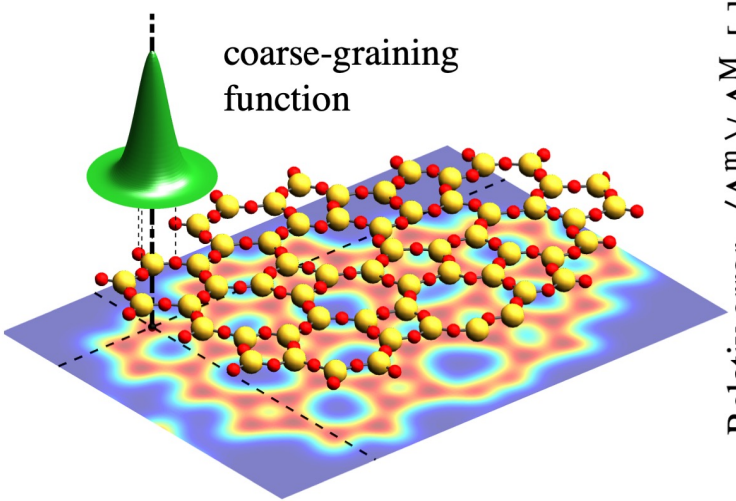
Coulomb:

- PPPM
- Wolf truncation

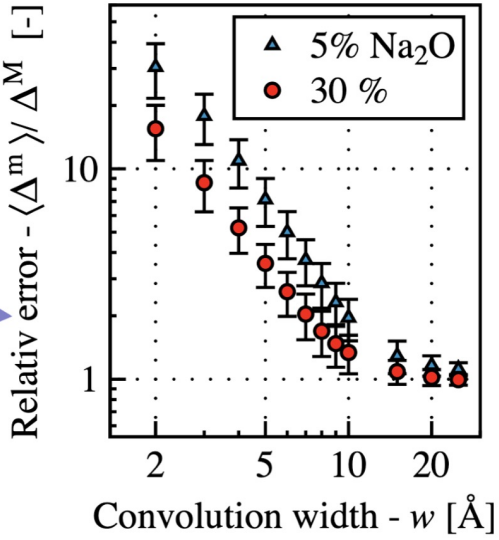
Resistance of Silicate Glasses

From discrete to continuum / CG

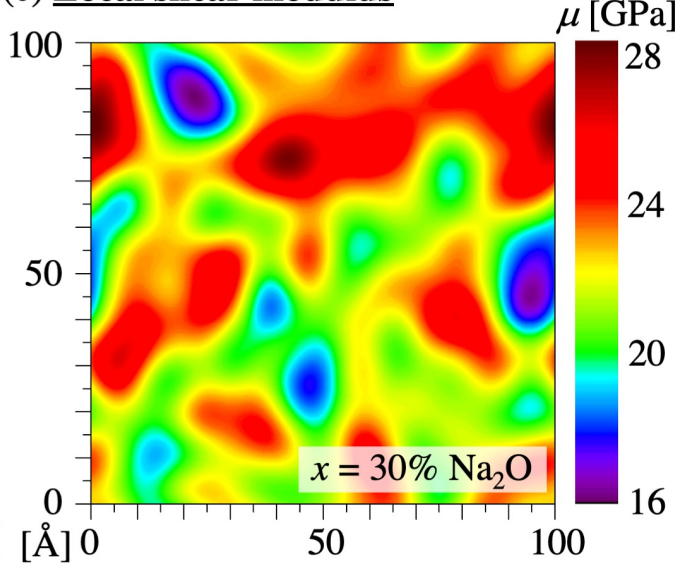
(a) **Gaussian convolution**



(b) **Local error**



(c) **Local shear modulus**

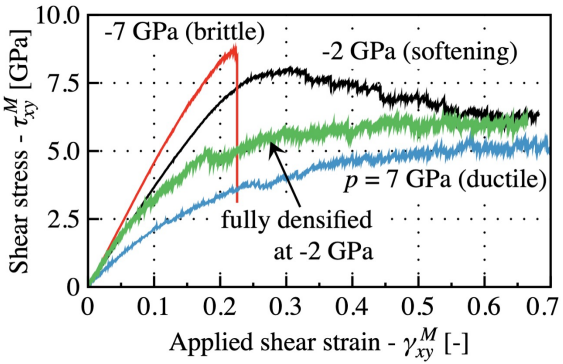


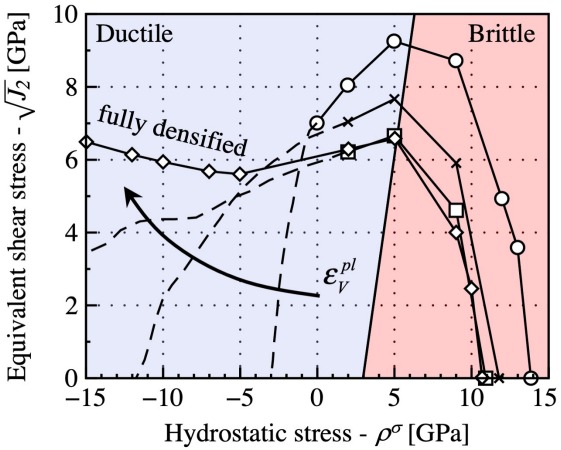
Resistance of Silicate Glasses

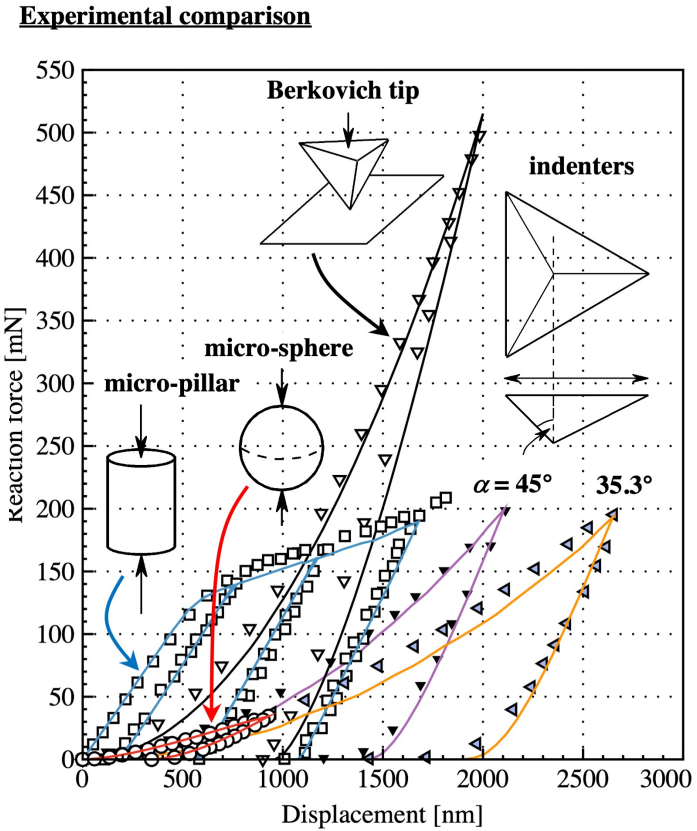
(Kermouche et al., 2016)

Ductile behavior / Yield criteria

Yield strength: 5-7 GPa







Micro-pillar

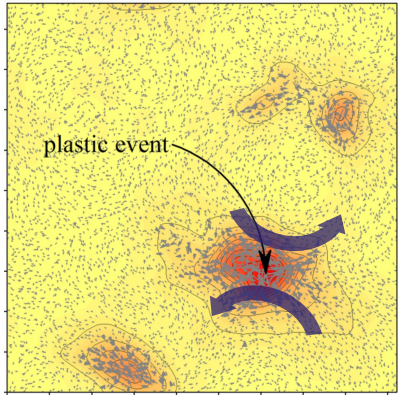
- pure SiO_2
- ambient temperature
- 4-6 µm size

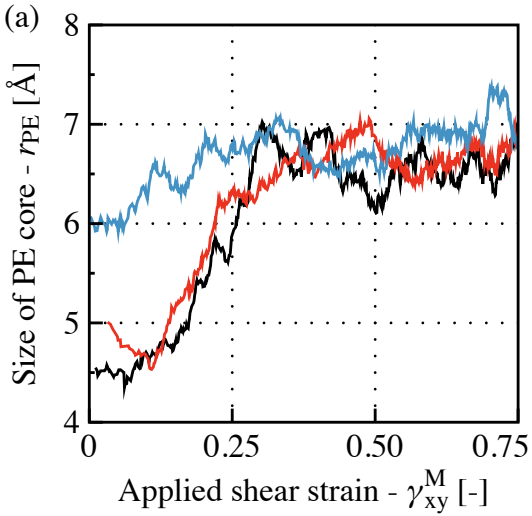
Resistance of Silicate Glasses

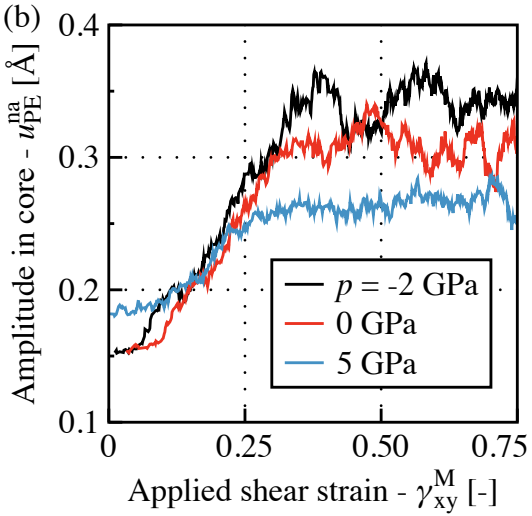
Ductile behavior / plastic events

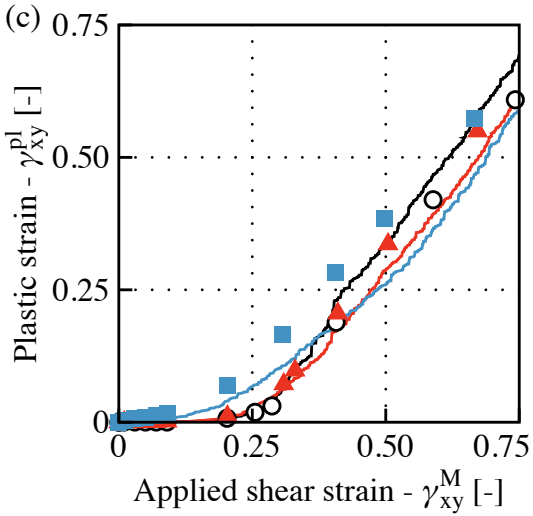
Plastic event (STZ)

- elliptic shape
- exponential decay
- characteristic size







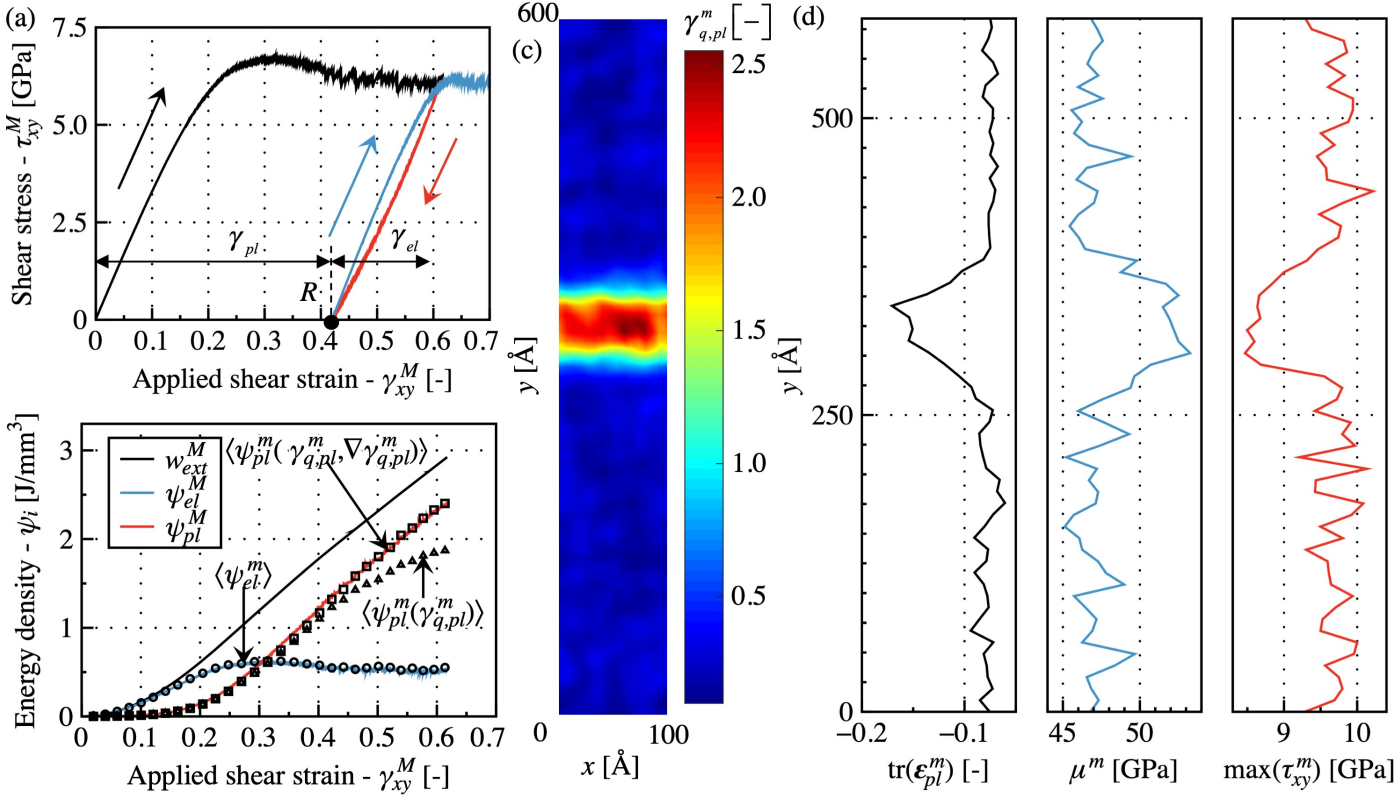


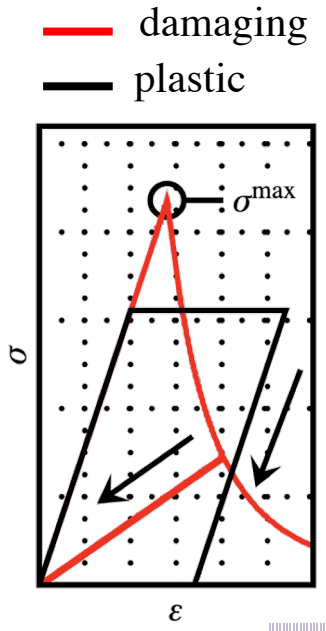
(Molnár et al, 2017)

Resistance of Silicate Glasses

Ductile behavior / shear banding

$$\left\langle \psi_{pl}^{m} \right\rangle = \frac{1}{V} \int_{\Omega} \left[\int_{t} \sigma^{m} : \varepsilon_{pl}^{m} \, dt + l_p^2 \sigma^{m} \left| \nabla p_{eq} \right|^2 \right] d\Omega$$



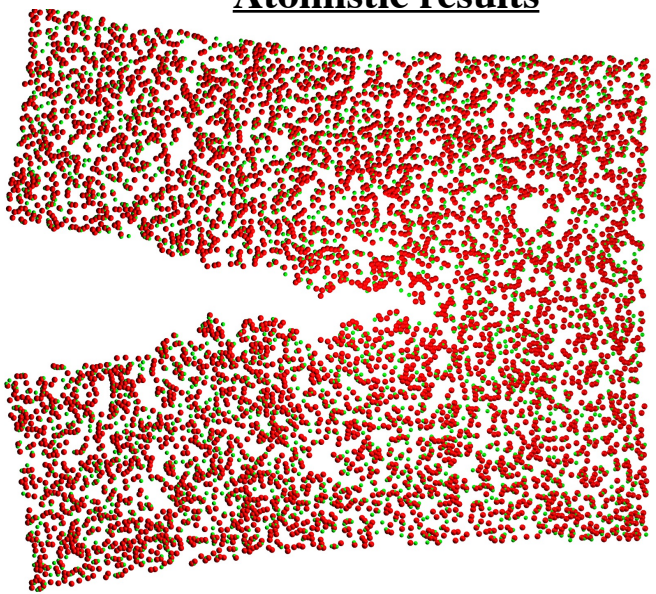


Resistance of Silicate Glasses

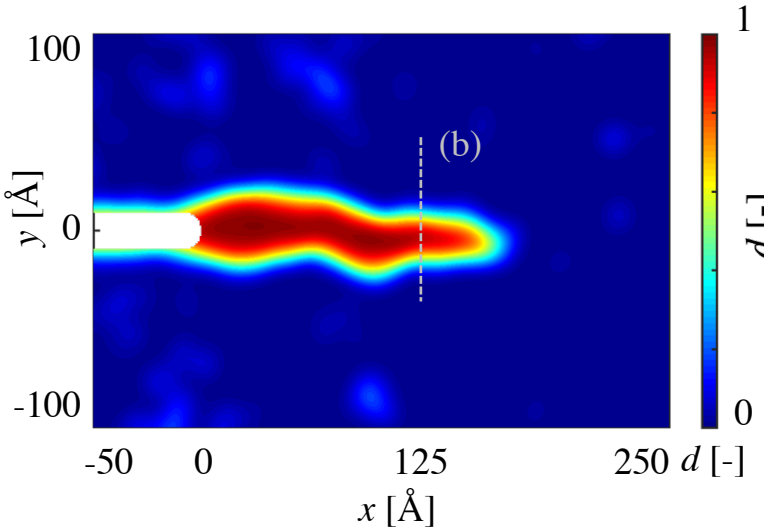
(Molnár & Barthel, submitted to PRL)

Fracture

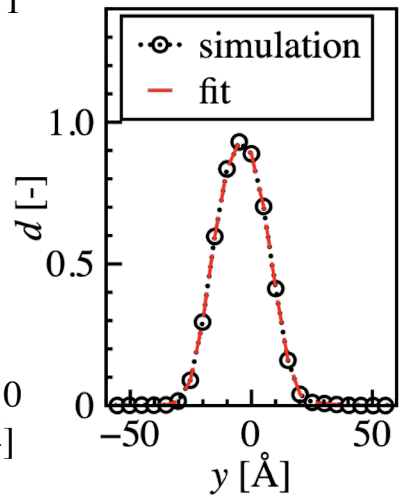
Atomistic results



Damage topology



Profile

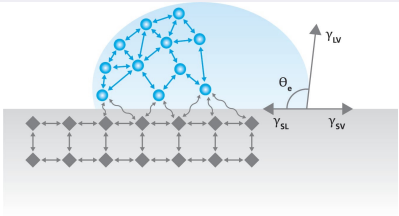


$$\Pi(\mathbf{u},d)=\int_\Omega (1-d)^2\,\psi_0^+(\boldsymbol{\varepsilon},\mathbf{C}_0)+\psi_0^-(\boldsymbol{\varepsilon},\mathbf{C}_0)\,d\Omega+\frac{g_c}{c_\omega}\int_\Omega\left(\frac{\omega(d)}{l_c}+\frac{l_c}{2}|\nabla d|^2\right)d\Omega$$

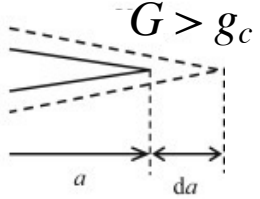
Resistance of Silicate Glasses

(Molnár & Barthel, submitted to PRL)

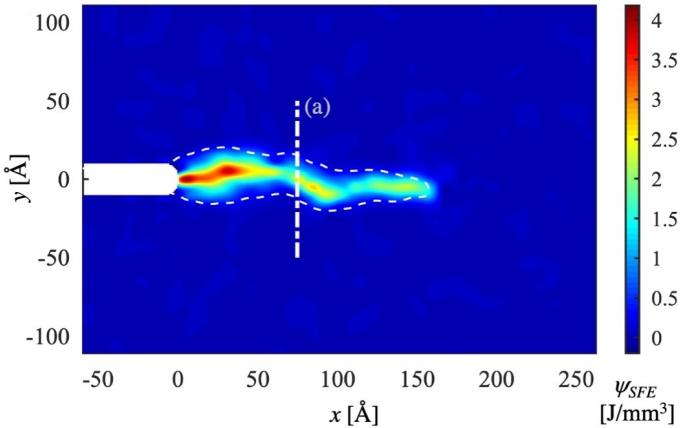
Fracture



Free Surface Energy $\ll$ Fracture Toughness

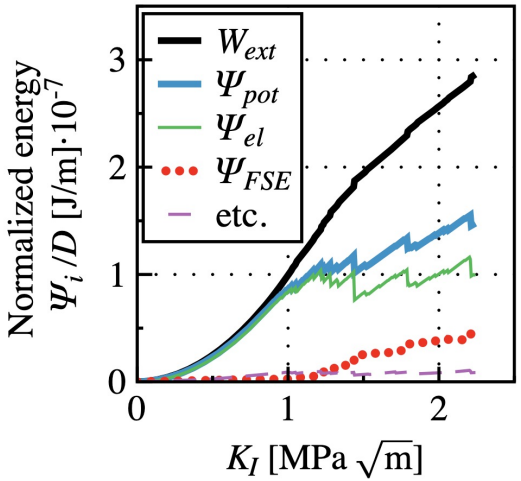


Free surface energy

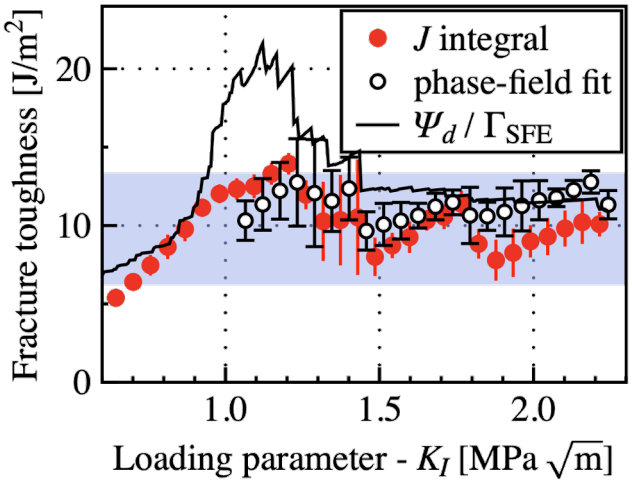


$$\psi_{FSE} = \psi_{pot} - \psi_{el}(\varepsilon)$$

Energy equilibrium



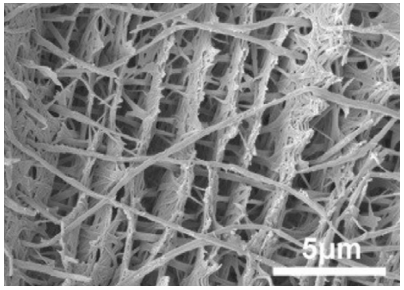
Fracture toughness

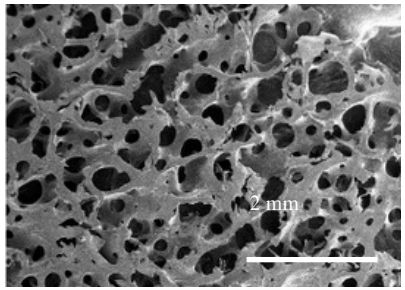


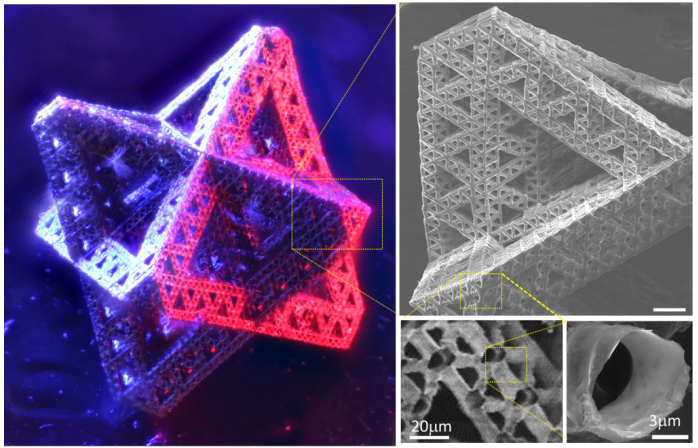
Architected Materials

Mechanical metamaterials

Natural examples





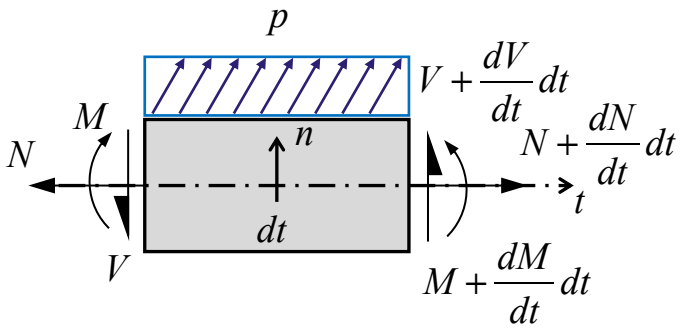


(Lin et al., 2021)
(Kytyr et al., 2012)

Man-made examples

(Zheng et al, 2015)

Euler-Bernoulli beam theory



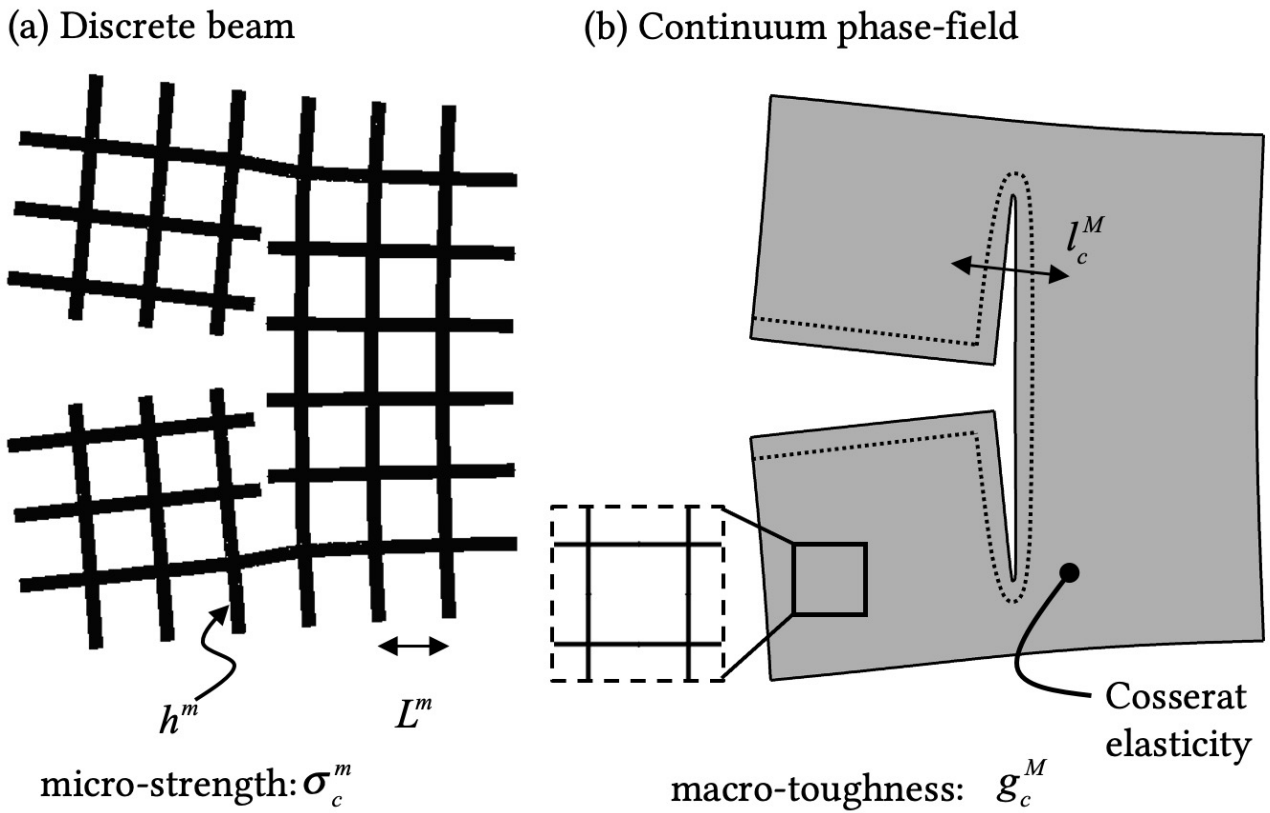
Modelling assumptions

- beams are flawless
- no stress concentration at joints
- $\sigma_t < \sigma_c^m$

Architected Materials

(Molnár & Réthoré, submitted to JTCAM)

Strategy

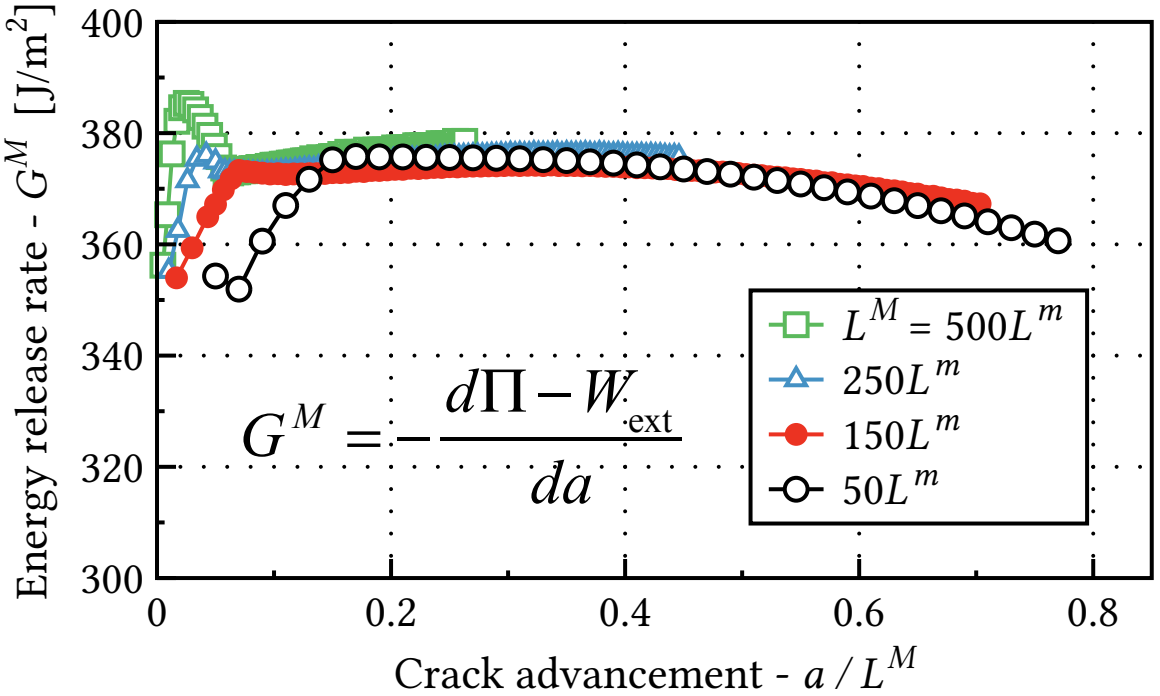


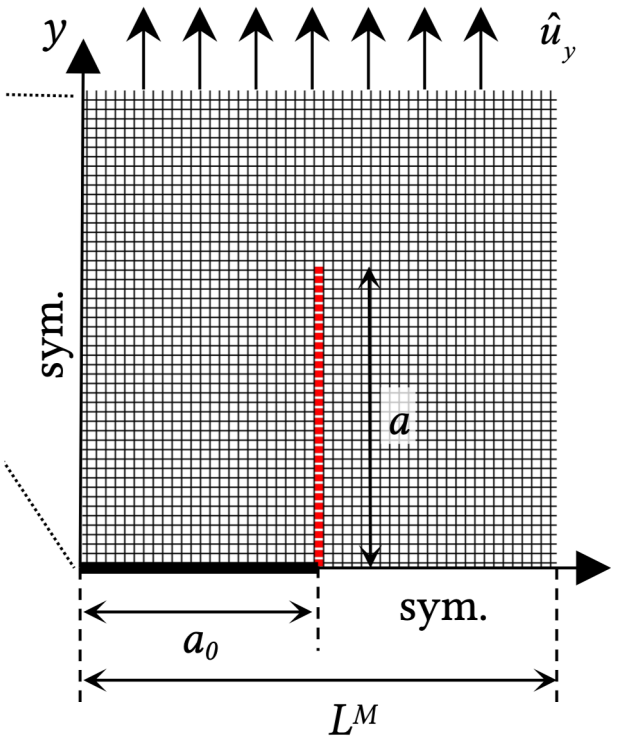
- Critical load
- Fracture topology
- Various loading

Architected Materials

(Molnár & Réthoré, submitted to JTCAM)

Existence of a unique toughness





Continuum model

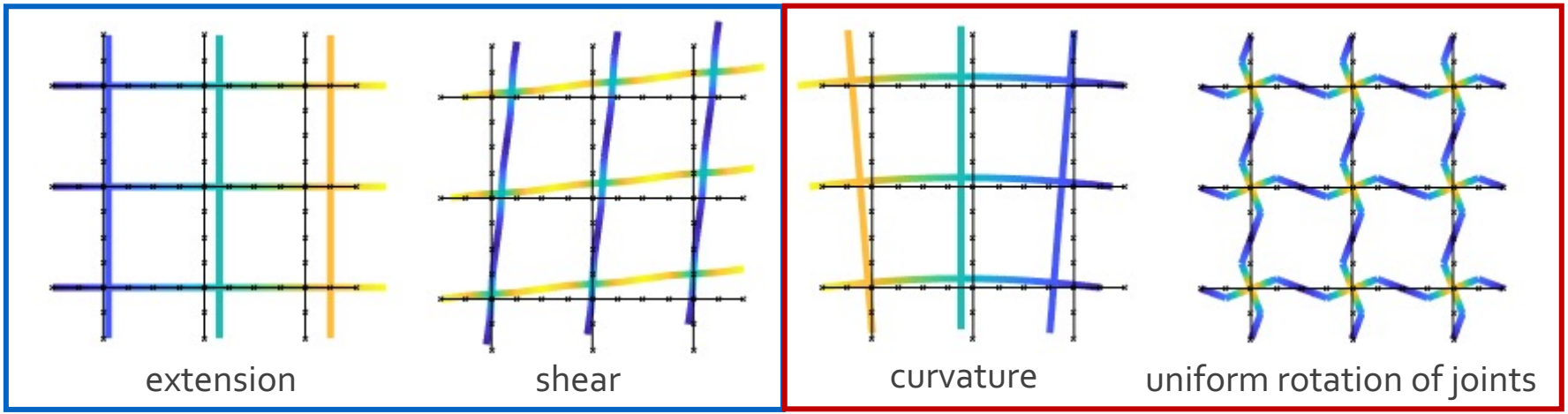
(Molnár & Réthoré, submitted to JTCAM)

Cosserat phase-field fracture

New DOF: rotation ϕ

New deformations

(Cosserat & Cosserat, 1909)



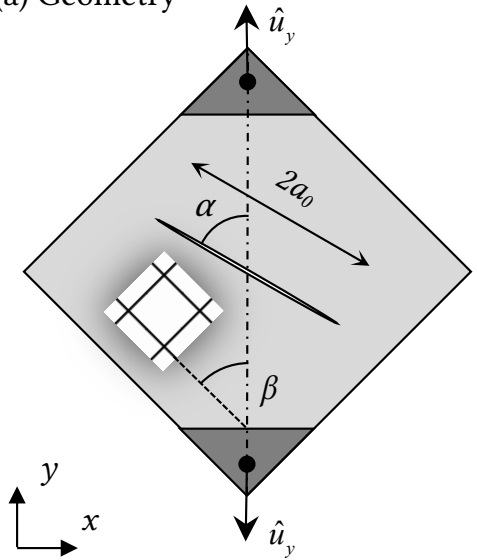
$$\Pi(\mathbf{u},d)=\Psi\left(\mathbf{u},\phi,g_{ij}\left(d_i\right)\right)+\sum_{i=1}^{2}\frac{3g_{c,M,i}}{8l_{c,M,i}}\int_{\Omega}\left(d_i+l_{c,M,i}^{2}\left|\nabla d_i\right|^{2}\right)d\Omega$$

Architected Materials

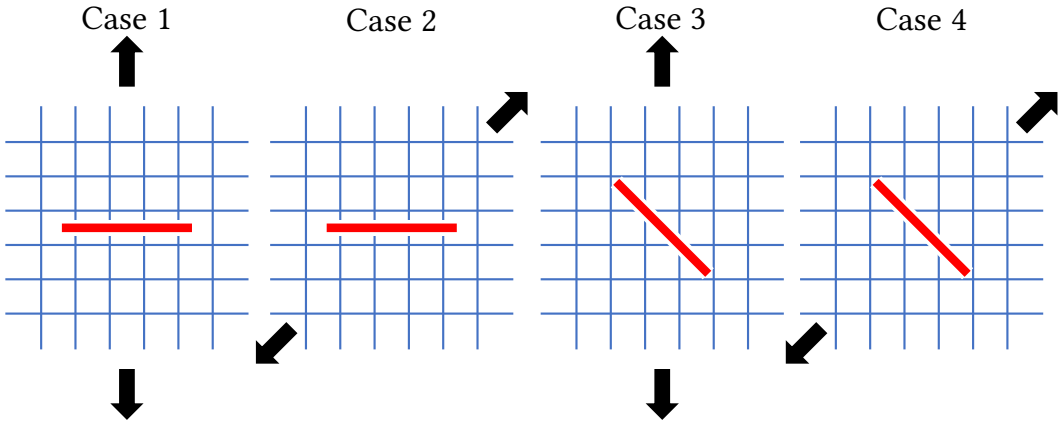
(Molnár & Réthoré, submitted to JTCAM)

Experimental validation

(a) Geometry



(b) Orientations

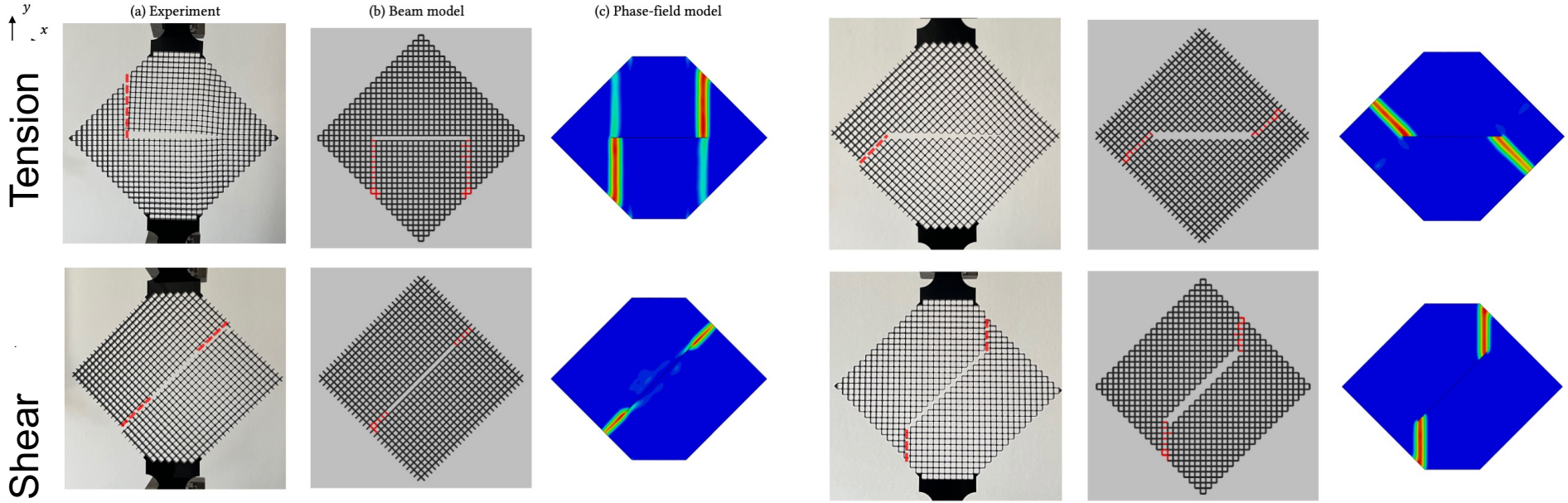


	Case 1	Case 2	Case 3	Case 4
Crack/Loading (α):	90°	45°	45°	90°
Structure/Loading (β):	90°	45°	90°	45°
Crack/Structure :	0°	0°	45°	45°

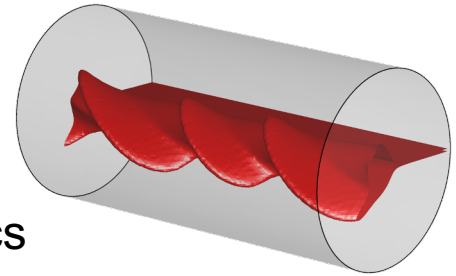
Architected Materials

(Molnár & Réthoré, submitted to JTCAM)

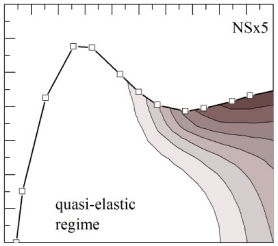
Experimental validation

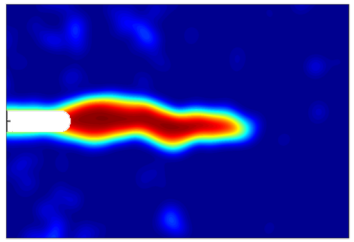


Contributions



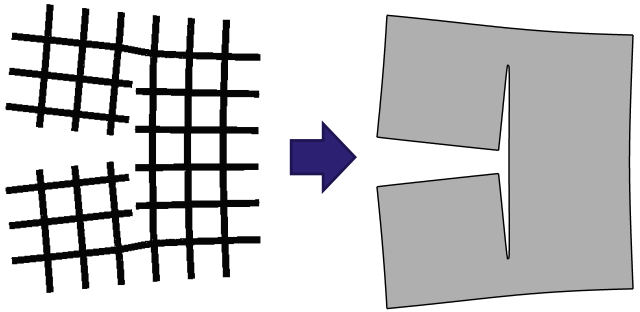
1. **Regularization** allows us to model **real** physical phenomena
2. Irwin's length – phase-field length – characteristic crack length
3. Connection of **limiting velocity** and **regularization** in dynamics





4. **Length scales** form the **atomic scale** for glasses
5. **Damage** correlates **free** and **fracture** surface energies

6. Periodic **beam lattices** have a **unique fracture toughness**
7. **Cosserat** theory is necessary and sufficient.



Contributions

Open-source phase-field implementation

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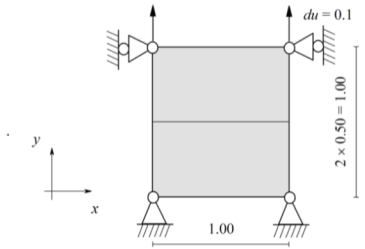
Fracture modeling with phase field method

1. Simple tension with 2 elements

The tutorial presents a simple conversion between the input file generated by ABAQUS and the use of the new UEL.

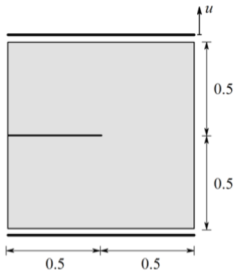
The instructions can be downloaded from here. While the files used and created through the tutorial are accessible from this link.



2. Single edge notched sample & MATLAB converter

The tutorial presents a single edge notched sample and how to develop simple models using ABAQUS/CAE and convert them with a MATLAB script (still in Beta testing stage).

It contains a FORTRAN script with both triangular and square elements. The instructions are shown here. While the files used and created through the tutorial are accessible from this link.



Movie | Files

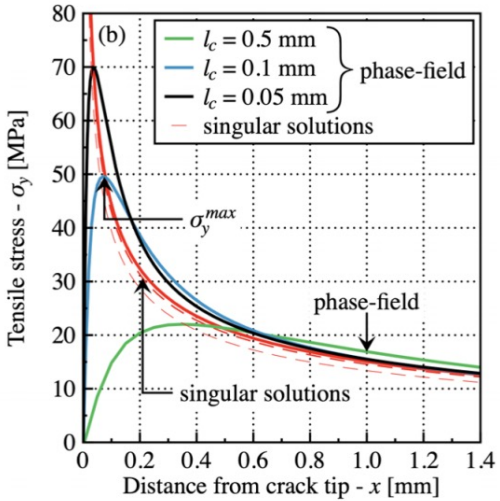
Please visit

www.molnar-research.com

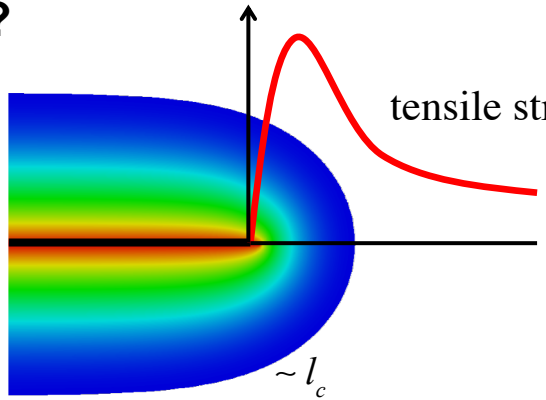
gergely.molnar@insa-lyon.fr

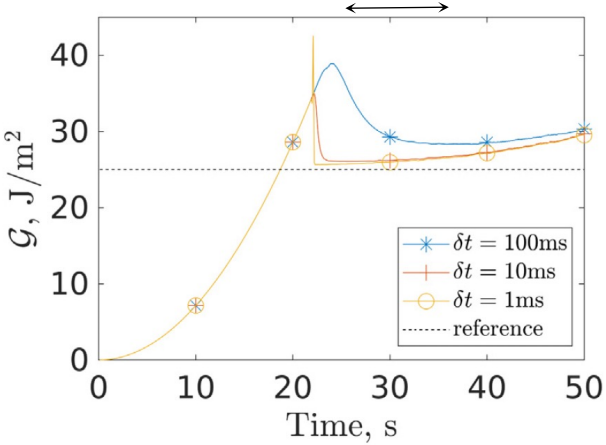
Perspectives

Measurement of l_c ang g_c?

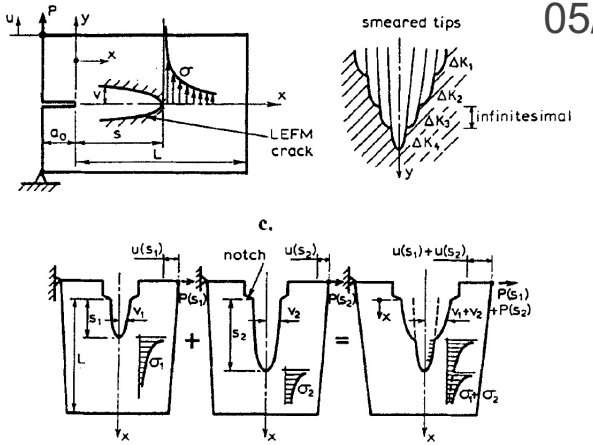


(Molnár et al., 2020)





(Kolditz et al., 2024)



(Bažant & Beissel, 1994)

Thomas Duminy

05/2025

Perspectives

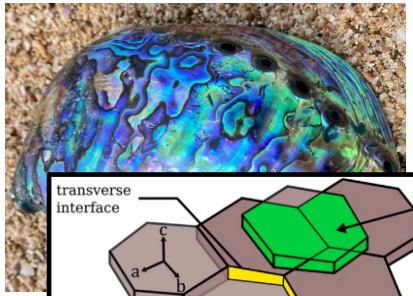
Atomic-scale modeling

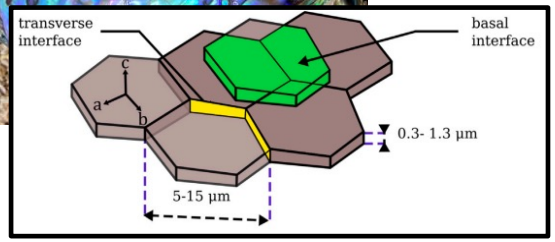
with A. Doitrand
S. Meille

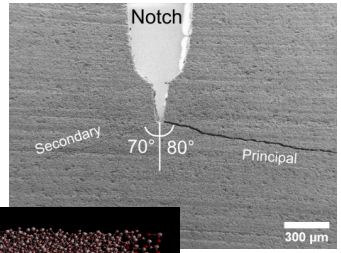
MatéIS
Matériaux Ingénierie et Science
UMR 5510

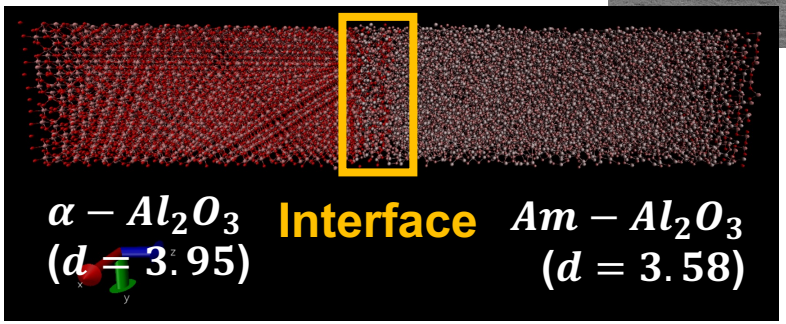
Benjamin Bert
10/2023

Nacre-like alumina

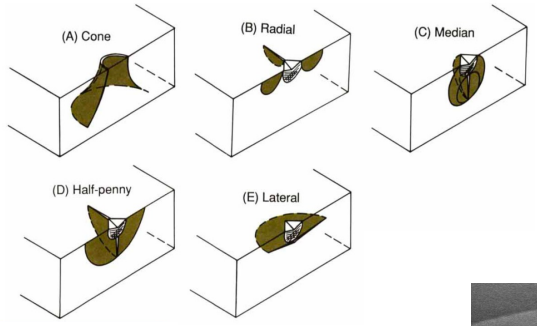




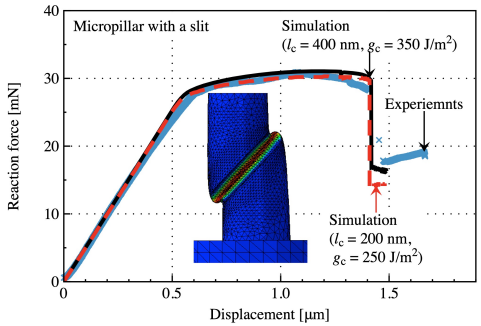


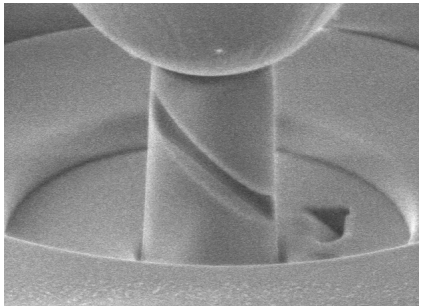


Indentation resistance of silicate glasses



(Cook & Pharr, 1990)





(Guillonneau et al., 2022)

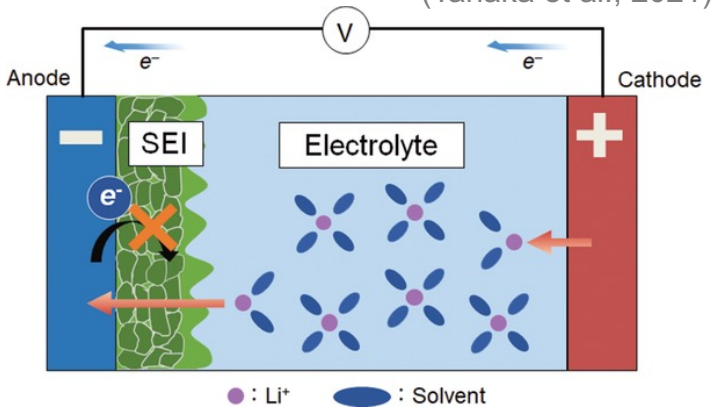
Souhail Chaouch
05/2025

anr
GaLAaD

Perspectives

Si based battery optimization

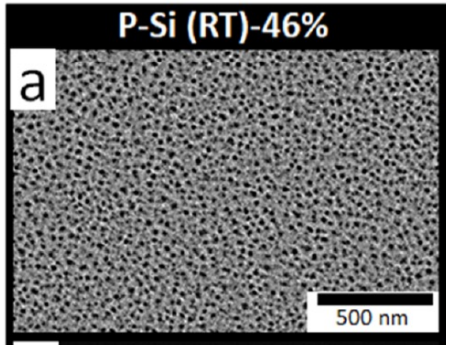
(Tanaka et al., 2021)



with N. Blal
D. Machon

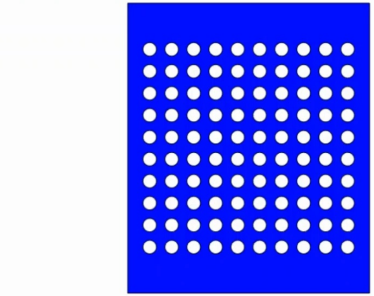
Tom Guisard
10/2024

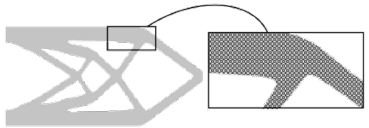
Post-treatment



(Abdelouhab et al., 2024)

Optimization





Advantages

- 10x capacity
- natural, abundant, cheep
- environmentally friendly

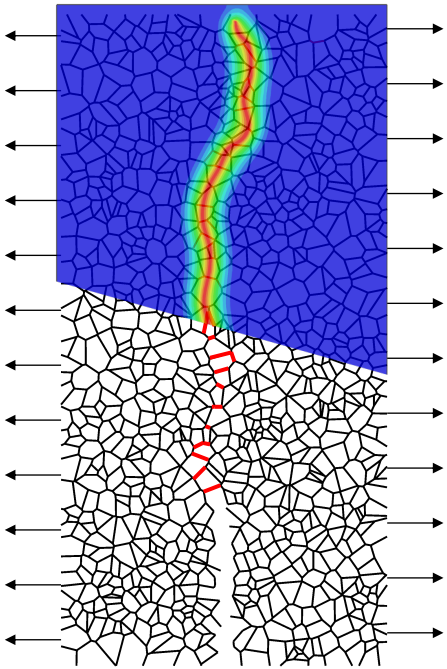
Disadvantages

- 300% volume expansion
- few charges (delamination)

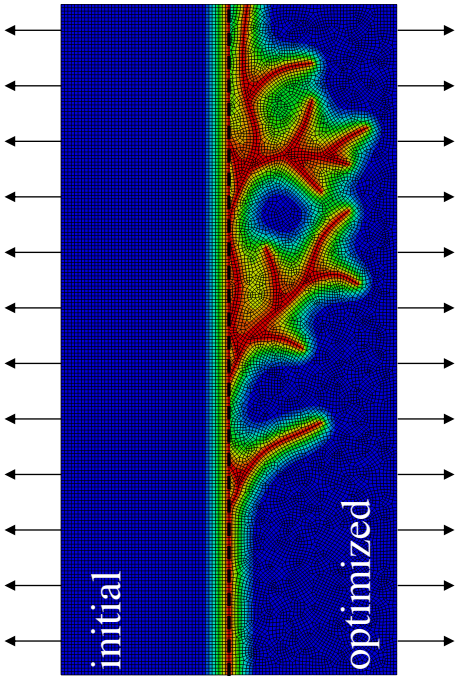
Perspectives

Optimization for toughness

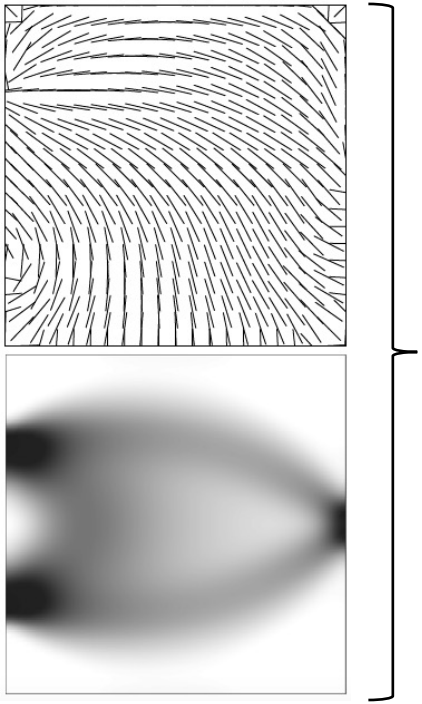
(a) **Homogenization**



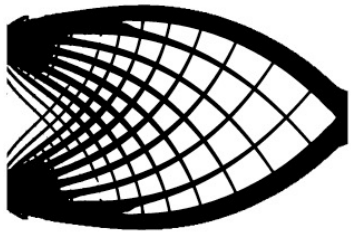
(b) **Optimization**



(c) **Rendering and testing**



final structure



(Geoffroy-Donders, 2018)

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Mentors



PhD and postdocs




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LaMCoS
Laboratoire de Mécanique des Contacts et des Structures
UMR 5259

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My Family

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Aurélien Doitrand

Université Claude Bernard Lyon 1 — INSA

N° Identificateur — Année 2025

HABILITATION A DIRIGER DES RECHERCHES

présentée devant

l'Institut National des Sciences Appliquées de Lyon
et l'Université Claude Bernard Lyon I

Contribution à l'étude de l'amorçage de fissures dans les matériaux fragiles

par

Aurélien Doitrand

Soutenance prévue le 28 Mars 2025

Composition du jury

Rapporteurs :	Djimédo Kondo	IJLRA, Sorbonne Université
	Christophe Bois	I2M, Université de Bordeaux
	Sylvain Drapier	LGF, Ecole des Mines de Saint-Etienne
Examinateurs :	Julien Réthoré	GeM, Université de Nantes
	Thouraya Baranger	LMC2, Université Claude Bernard Lyon I
	Nathalie Godin	MATEIS, INSA de Lyon
	Sylvain Meille	MATEIS, INSA de Lyon

Laboratoire MATéIS : MATériaux, Ingénierie et Science - UMR 5510

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Save the date!

28/03/2025